



23rd International Symposium on

**NON-OXIDE AND
NEW OPTICAL
GLASSES
(ISNOG)**

June 14–17, 2026

DGI Byen, Copenhagen,
Denmark

General information

Venue: DGI Byen - Tietgensgade 65, 1704 København V

Website: <https://www.isnog.bio.aau.dk/>

Food and drinks

As part of the registration fee, we offer a welcome reception at 16:00 on Sunday June 14, daily lunches and coffee breaks on Monday through Wednesday June 15-17, as well as a conference dinner at 18:00 on Tuesday June 16. All events take place at the DGI Byen venue.

Conference meeting rooms

Auditorium Sankt Hans Torv: 221 seats (ground floor)

Enghave Plads og Kødbyen: 116 seats (second floor)

Tivoli og Vesterbros Torv: 95 seats (second floor)

Duration of presentations (incl. Q&A)

Plenary talk: 35 min

Invited talk: 25 min

Oral contribution: 15 min

Posters

Size of board: 100 x 215cm. Mounting with mounting putty or tape.

Conference chairs

Morten M. Smedskjær (Aalborg University)

Yuanzheng Yue (Aalborg University)

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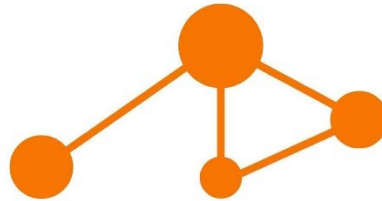
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Welcome message

The **International Symposium on Non-Oxide and New Optical Glasses (ISNOG)** has become a pivotal event in the field of glass science and technology. With the rapid emergence of new types of non-oxide glasses and the discovery of their unique functionalities, the scope of ISNOG has broadened significantly. While originally centered on non-oxide glasses and their optical properties, the symposium now reflects major advancements across a range of glass systems and their novel physical behaviors. ISNOG serves as a key platform for academic exchange, technological innovation, and international collaboration within the global glass research community.

ISNOG has been held approximately biennially since its inception in 1981 in Cambridge, UK. It has been hosted in numerous countries, including the USA, France, Japan, Australia, Germany, Brazil, the Czech Republic, India, China, Korea, Russia, and Canada. We are happy that you are joining us for the 23rd ISNOG in Copenhagen, Denmark, from June 14–17, 2026. This season offers more than 17 hours of daylight, and the symposium will be hosted at the centrally located DGI Byen, within walking distance of Copenhagen Central Station, various hotels and attractions such as Tivoli Gardens. Copenhagen is continuously rated among the happiest and most liveable cities in the world.

Like previous conferences, the 23rd ISNOG is bringing together scientists from around the world interested in the chemistry, physics, optics, mechanics, and engineering of non-oxide and new optical glass materials as well as both experimental and computational techniques for their advanced characterization. The conference is organized into five technical symposia.

We are happy to welcome industrial researchers, engineers, experts from academia, and students to promote discussions and exchanges of knowledge. Through plenary sessions and both oral and poster presentations, we aim to create an open atmosphere that allows new collaborations and friendships to be formed and ideas to be shared and discussed.

Morten M. Smedskjær, Yuanzheng Yue
Conference chairs

Venue

DGI Byen - Tietgensgade 65, 1704 København V

Conference meeting rooms

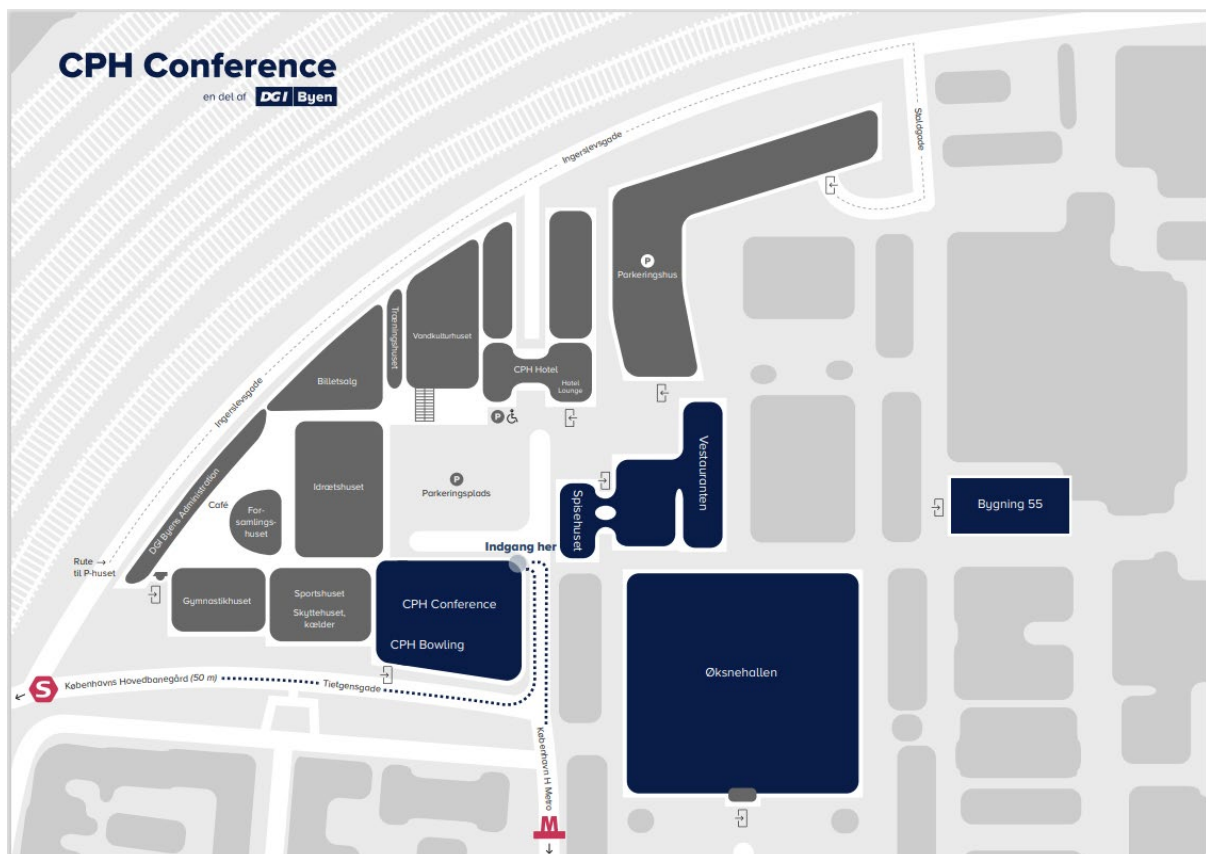
Auditorium Sankt Hans Torv: 221 seats (ground floor)

Enghave Plads og Kødbyen: 116 seats (second floor)

Tivoli og Vesterbros Torv: 95 seats (second floor)

Poster sessions and coffee breaks

Lobby on ground floor



Symposia

1. *Fundamentals of glasses: formation, structure and physical properties*
2. *Glasses for photonic devices, lasers, data storage, and processing tools*
3. *Glasses for health and green energy technology*
4. *New non-oxide glasses, hybrid glasses and phase-change materials*
5. *Simulations and predictive modelling of glasses*

Plenary speakers

Matthias Wuttig, RWTH Aachen University, Germany
Unraveling the origin of non-Zachariasen glasses

Lili Hu, Shanghai Institute of Optics and Fine Mechanics, CAS, China
Manipulation of spectroscopic properties of active ions in glass via local structure

Heike Ebendorff-Heidepriem, Adelaide University, Australia
Reinventing soft glasses and fibres through adding crystal particles, tuning fibre microstructure or processing in microgravity

Sabyasachi Sen, Department of Materials Science and Engineering, University of California, Davis, USA
Atomistic Understanding of Structure, Relaxation and Related Phenomena in Chalcogenide Glasses and Glass-Forming Liquids

Sebastian Leukel, Development SCHOTT AG, Germany
From Augmented Reality to Laser Fusion: Glass at the Core of Future Technologies

Jianrong Qiu, Zhejiang University, China
Ultrafast laser induced order/disorder changes and applications

Program - Sunday June 14

Join us for the **Welcome Reception** from **16:00 to 18:00** at DGI Byen on Sunday June 14th. The reception will be a standing reception with a light menu and one drink included.

Location: Østerbro Restaurant (third floor) at DGI Byen - Tietgensgade 65, 1704 København V

Registration also takes place in the same location.

Program - Monday June 15

(plenary/invited speakers written in blue font)

Plenary session (room: auditorium)

Session chair: Yuanzheng Yue (assistant: Sidsel M. Johansen)

- 08:00 Morten M. Smedskjær: *Welcome*
- 08:10 Matthias Wuttig: *Unraveling the origin of non-Zachariasen glasses*
- 08:45 Lili Hu: *Manipulation of spectroscopic properties of active ions in glass via local structure*

Coffee break and poster session

9:20 - 9:50

Symposium 2 (room: auditorium)

Session chair: Xianghua Zhang (assistant: Zhencai Li)

- 09:50 Shibin Jiang: *High Peak Power Fiber Lasers*
- 10:15 Nilanjana Shasmal: *Lead-Free Perovskite-Doped Glasses: Promising Materials for White Light Emission*
- 10:30 He Shasha: *Tunable dual-band photoluminescent CsPbBr₃ quantum dots in glass for light-emitting applications*
- 10:45 Yiguang Jiang: *Preparation and Application of Mid-infrared Fluoride Glass Fiber*
- 11:00 Dezhi Tan: *Regulation of micro/nano-structures and photonic functionalities of glass*
- 11:25 Yanqing Fu: *Chalcogenide Glass Fibers and Their Optoelectronic Sensing Applications*
- 11:40 Alexis Duval: *Facile and Quantitative Determination of Glass Redox State*

Symposium 4 (room: Enghave Plads og Kødbyen)

Session chair: Jingwei Hou (assistant: Johan F. S. Christensen)

- 09:50 Satoshi Horike: *Molecular doping into the metal-organic framework glasses for functional materials*
- 10:15 Hoi Ri Moon: *Designing Vitriifiable Metal–Organic Frameworks through Coordination and Molecular Dynamics*
- 10:40 Sebastian Henke: *Chemical Approaches to Tuning the Structure and Properties of Hybrid Glasses*

- 11:05 [Guillermo M. Espallargas](#): *Iron-based zeolitic imidazolate framework glasses and beyond: from multi-structural phase transitions to direct synthesis*
- 11:30 [Alexander Knebel](#): *Taking a Magnifying Glance Through the MOF-Glass*

Symposium 1 (room: Tivoli og Vesterbros Torv)

Session chair: Alex Hannon (assistant: Peter G. Jensen)

- 09:50 [Seong H Kim](#): *Infrared Light–Glass Interactions: Insights into Network Structure*
- 10:15 [Collin Wilkinson](#): *Hybrid Methods for Predicting Vibrational Properties of Glasses*
- 10:40 [Elsebeth J. Pedersen](#): *Structure of Hydrated Borate Glasses*
- 10:55 [Jinwook Jang](#): *Compositional Effect on Chemical Strengthening and Mechanical Properties of $\text{SiO}_2\text{--B}_2\text{O}_3\text{--Al}_2\text{O}_3\text{--Na}_2\text{O}$ Glass*
- 11:10 [Sidsel M. Johansen](#): *Correlating structural relaxation and fracture toughness in aluminoborosilicate glasses*
- 11:25 [Liu Wei](#): *Effect of B_2O_3 substitution for Al_2O_3 on crystallization behavior, microstructure, and mechanical properties of forsterite-based glass-ceramics*
- 11:40 [Sourav Sahoo](#): *Indentation Deformation Mechanisms of Intermediate Calcium Aluminoborosilicate Glasses*

Lunch break

12:00 - 13:15

Symposium 2 (room: auditorium)

Session chair: Lili Hu (assistant: Suresh Bishnoi)

- 13:15 [Laetitia Petit](#): *Rare-Earth doped Glasses for (bio)Photonic Systems*
- 13:40 [Andrea S. S. de Camargo](#): *From Structure to Function: RE-doped Fluoride-Phosphate Glasses for Advanced Optical Applications*
- 14:05 [Lothar Wondraczek](#): *Optical Fiber Preform Materials: Novel Approaches in Powder Doping for Versatile Fiber Architectures in Medical and Industrial Photonics*
- 14:20 [Chen Tian](#): *$\text{CaTa}_2\text{O}_6/\text{Al}_2\text{O}_3$ composite ceramics prepared via crystallization from $\text{CaO-Ta}_2\text{O}_5\text{-Al}_2\text{O}_3$ glasses for highly-sensitive luminescent temperature sensing*
- 14:35 [Jian Ruan](#): *NIR-II emitting Ni^{2+} activated glass-ceramics prepared via controlled crystallization from $\text{MTa}_2\text{O}_5\text{-Al}_2\text{O}_3$ ($M=\text{Ca, Sr or Ba}$) glasses*

Symposium 4 (room: Enghave Plads og Kødbyen)

Session chair: Hoi Ri Moon (assistant: Xiaoyi Xu)

- 13:15 [Jingwei Hou](#): *Metal Organic Framework Glass Composites*
- 13:40 [Ang Qiao](#): *Magnetism Evolution Induced by Structural Disorder in an Fe-Based Zeolitic Imidazolate Framework*
- 14:05 [Søren S. Sørensen](#): *Continuous structure and property tuning of metal-organic framework glasses*
- 14:20 [Samraj Mollick](#): *Ion Exchangeable Hybrid Glasses for Selective Mineral Harvesting from Seawater*
- 14:35 [Yong Li](#): *Disorder-Enabled Isotropic Lithium Diffusion in Zeolitic Imidazolate Framework Glasses*

Symposium 1 (room: Tivoli og Vesterbros Torv)

Session chair: Giulio Monaco (assistant: Søren C. J. Hansen)

- 13:15 [Kristine Niss](#): *Experimental test of the isomorph theory: a step towards understanding glass-forming liquids*
- 13:40 [Jun-Qiang Wang](#): *Critical roles of activation entropy in relaxation and glass transition*
- 14:05 [Tina Hecksher](#): *Broadband Shear Mechanical Measurements on Glass-forming Materials*
- 14:20 [Hanna M. Wenzel](#): *Structure determination in molecular amorphous solids with nonlinear optical properties*
- 14:35 [Kenji Shinozaki](#): *Pre-Existing Bicontinuous Structures in Oxyfluoride Glass Melts and Their Role in Ultrafast Nucleation Revealed by Chromatic Topological and Coarse-Grained Analyses*

Coffee break and poster session

15:00 - 15:30

Symposium 2 (room: auditorium)

Session chair: Pierre Lucas (assistant: David L. Christensen)

- 15:30 [Yong Gyu Choi](#): *Te-based chalcogenide glasses for use as thermal-imaging lenses: Momentum and potential*
- 15:55 [Petr Nemeč](#): *Temperature-dependent optical functions of selected Ge-Sb-Se bulk chalcogenide glasses determined using spectroscopic ellipsometry*
- 16:10 [Wei Zhang](#): *Chalcogenide photonic devices and application in complex refractive index sensing*

Symposium 4 (room: Enghave Plads og Kødbyen)

Session chair: Shuai Wei (assistant: Andreas S. Andersen)

- 15:30 Robert Maass: *Hierarchical microstructures in metallic glasses – are they real?*
- 15:55 Isabella Gallino: *On the nature of the glass transition in metallic glasses studied via fast scanning calorimetry*
- 16:20 Yelim Lee: *Design Strategies for Vitrification in Rare-Earth Carboxylate-Based Coordination Polymers*

Symposium 1 (room: Tivoli og Vesterbros Torv)

Session chair: Andrea S. S. de Camargo (assistant: Sourav Sahoo)

- 15:30 Jihong Zhang: *Plasma melting $Al_2O_3-R_xO_y$ binary aluminate glass and transparent ceramics microspheres*
- 15:55 Jinjun Ren: *Crystallization Mechanism of Fluorine-Oxygen Glasses – Elucidated by Solid-State NMR Spectroscopy*
- 16:20 Néstor Merino-Díez: *Growth of secondary phases on calcium aluminosilicate glass surfaces*

Program - Tuesday June 16

(plenary/invited speakers written in blue font)

Plenary session (room: auditorium)

Session chair: Morten M. Smedskjær (assistant: Søren S. Sørensen)

- 08:00 [Heike Ebendorff-Heidepriem](#): *Reinventing soft glasses and fibres through adding crystal particles, tuning fibre microstructure or processing in microgravity*
- 08:35 [Sabyasachi Sen](#): *Atomistic Understanding of Structure, Relaxation and Related Phenomena in Chalcogenide Glasses and Glass-Forming Liquids*

Coffee break and poster session

9:10 - 9:45

Symposium 2 (room: auditorium)

Session chair: Shibin Jiang (assistant: Søren S. Sørensen)

- 09:45 [Sen Qian](#): *The R&D of the High Light Yield and High Density Glass Scintillator for High Energy Physics Detectors*
- 10:10 [Chao Liu](#): *Lead-free halide nanocrystals in glass: tailoring luminescence for advanced optoelectronic applications*
- 10:35 [Guoping Dong](#): *Hybrid Glass Fiber and Its Optical Applications*
- 11:00 [Zhi Chen](#): *Ultrafast Laser 3D micro-nano Fabrication of Core Architectures for Glass-based Photonic Quantum Chips*
- 11:25 [Sachin Kumar](#): *Tellurite fibre fabrication with NV-containing diamond particles using an interface-based approach*
- 11:40 [Chao Ruan](#): *Perovskite nanocrystals in glass for high efficiency and ultra-high resolution dynamic holographic multicolor display*

Symposium 4 (room: Enghave Plads og Kødbyen)

Session chair: Jianrong Qiu (assistant: Søren C. J. Hansen)

- 09:45 [Changgui Lin](#): *Chalcogenide Glasses for Advanced Optoelectronic Applications*
- 10:10 [Shiliang Kang](#): *Advanced chalcogenide glasses and their optoelectronic sensing applications*
- 10:35 [Chengwei Gao](#): *IR transparent and flexible chalcogenide organic glass*

- 11:00 [Linling Tan](#): *Development and Imaging Applications of Infrared Chalcogenide Glasses*
- 11:25 [Nguyen M. P. Truong](#): *Luminescence modulation in Tb/Yb codoped oxyfluoride glass and their glass-ceramic counterparts*
- 11:40 [Yixi Wu](#): *Tough transparent glass ceramics for multi-mode programmable dynamic tunable persistent luminescence via phase engineering*

Symposium 1 (room: Tivoli og Vesterbros Torv)

Session chair: [Jincheng Du](#) (assistant: [Johan F. S. Christensen](#))

- 09:45 [Jeppe Dyre](#): *The material-time concept in physical aging*
- 10:10 [Ziqiang Chen](#): *Geological timescales' aging effects of lunar glasses*
- 10:25 [Ankit Singh](#): *Atomic-scale simulations of the mechanics of real-world glasses at experimentally accessible time-scales*
- 10:50 [Giulio Monaco](#): *Shaping Glasses with X-rays*
- 11:15 [Jens Moesgaard](#): *Elucidating the features of the Boson peak to expand upon the understanding of amorphous phase-change materials*
- 11:30 [Beatrice Baraldi](#): *In-Situ XRD Tracking of Structural Changes in Metallic Glasses During Thermal Scans*

Lunch break

12:00 - 13:15

Symposium 2 (room: auditorium)

Session chair: [Heike Ebendorff-Heidepriem](#) (assistant: [Elsebeth J. Pedersen](#))

- 13:15 [Xianghua Zhang](#): *Infrared optics with gradient refractive index based on chalcogenide glasses*
- 13:40 [Shixun Dai](#): *Recent Advances in Chalcogenide Glasses and Acousto-Optic Devices: From Structure–Property Correlations to Low-Power, High-Performance Modulators*
- 14:05 [David Le Coq](#): *Femtosecond laser writing of mid-infrared splitters in chalcogenide glasses*
- 14:20 [Virginie Nazabal](#): *Chalcogenide Glass Thin Films as Functional Materials for Infrared Photonic Water Pollution Sensors*

Symposium 4 (room: Enghave Plads og Kødbyen)

Session chair: Sabyasachi Sen (assistant: Anders M. Schade)

- 13:15 [Lothar Wondraczek](#): *Multiresponsive glasses*
- 13:40 [Pierre Lucas](#): *Towards Additive Manufacturing of Far-Infrared Optics*
- 14:05 [Shuai Wei](#): *Pressure–Temperature Driven Structural Evolution Across Polyamorphism in Phase-Change Materials*
- 14:30 [Yang Li](#): *Biomolecular Noncovalent Glasses: Fabrication Fundamental, Multifunctional Properties, and Emerging Applications*

Symposium 1 (room: Tivoli og Vesterbros Torv)

Session chair: Doris Möncke (assistant: Yong Li)

- 13:15 [Alex Hannon](#): *Bond Angles and The Structure of Vitreous Beryllium Fluoride*
- 13:40 [Ruilin Zheng](#): *Design and analysis of local structures of halide perovskite nanocrystals in glasses*
- 14:05 [Johann Troles](#): *Additive Manufacturing of ZBLAN Fluoride Glass via Fused Filament Fabrication*
- 14:20 [Qi Zhang](#): *Multiscale Structural Disorder in Glasses: Beyond Local Coordination Effects on Rare-Earth Ion Luminescence*

Coffee break and poster session

15:00 - 15:30

Symposium 2 (room: auditorium)

Session chair: Dezhi Tan (assistant: Zhencai Li)

- 15:30 [Félix Q. Martínez](#): *Non-conventional laser processing of glass*
- 15:55 [Zhencai Li](#): *White-light emission in zeolitic imidazolate framework glasses*
- 16:10 [Muhammad Umair](#): *Thermally and Optically Induced Johari Goldstein (JG) Relaxation in As_2Se_3*
- 16:25 [Iljung Yoon](#): *Composition-Dependent Viscoelastic Deformation Behaviors of Ge-Se-Te Glass for Use as Molded Lenses*

Symposium 3 (room: Enghave Plads og Kødbyen)

Session chair: Laeticia Petit (assistant: Peter G. Jensen)

- 15:30 [Leena Hupa](#): *Silicates: Paving the Way for Biodegradable Glasses in Tissue Regeneration*
- 15:55 [Qiang Fu](#): *Bioactive Glass for Improved Oral Care*
- 16:20 [Francesca Tallia](#): *Bouncy Bioglass – a new hybrid material for tissue regeneration*

Symposium 1 (room: Tivoli og Vesterbros Torv)

Session chair: Dominique de Ligny (assistant: Samraj Mollick)

- 15:30 [Philip S. Salmon](#): Bond counting strategies in an oxygen centric perspective on the structure of oxide glasses
- 15:55 [Mattias Edén](#): Predicting Contents of Non-Bridging Oxygens and Oxygen Triclusters in Aluminosilicate Glasses From ^{27}Al NMR Data
- 16:20 [Wei Zhang](#): Lanthanum Stabilized Cubic $\text{BaCl}_2:\text{Eu}^{2+}$ Nanocrystals in Glass with Enhanced Photoluminescence and Scintillation Performance for High-resolution X-Ray Imaging

Conference dinner

18:00 - 21:00

Program - Wednesday June 17

(plenary/invited speakers written in blue font)

Plenary session (room: auditorium)

Session chair: Yuanzheng Yue (assistant: Andreas S. Andersen)

08:00 [Sebastian Leukel](#): *From Augmented Reality to Laser Fusion: Glass at the Core of Future Technologies*

08:35 [Jianrong Qiu](#): *Ultrafast laser induced order/disorder changes and applications*

Coffee break and poster session

9:10 - 9:45

Symposium 3 (room: auditorium)

Session chair: Qiang Fu (assistant: David L. Christensen)

09:45 [Steve W. Martin](#): *Thin-Film Li Glassy Solid Electrolytes as a New Functionality for Glass Enabling High Energy Density Li All Solid State Batteries*

10:10 [Yanfei Zhang](#): *Engineering a Stable Electrode-Electrolyte Interface via Glass Structural Affinity for High-Performance All-Solid-State Lithium-Ion Batteries*

10:35 [Wengang Huang](#): *Engineering a Meltable MOF to Tune Liquid Transition and Promote Coenzyme Regeneration*

10:50 [Ashutosh Goel](#): *Structural origins of high MoO₃ solubility in peraluminous borosilicate glasses*

11:15 [Ziqiang Jia](#): *Improving Molybdenum Tolerance in Nuclear Waste Glasses: Compositional Modeling and Reduction Strategy*

Symposium 5 (room: Enghave Plads og Kødbyen)

Session chair: Kristine Niss (assistant: Sourav Sahoo)

09:45 [Stephen Elliott](#): *Chiral crystallization of amorphous tellurium*

10:10 [Konstantinos Konstantinou](#): *Nature of Electronic Excitations in Amorphous Phase-Change Memory Materials: Ge₂Sb₂Te₅*

10:25 [Lu Deng](#): *Revisiting the mechanisms of the phase separation and crystal growth by Molecular Dynamics*

10:50 [Aude Amari](#): *Identifying the limit of the Tool-Narayanaswamy formalism*

- 11:05 Nicholas Bailey: *Isomorph Invariance of mechanical properties of model glasses*
- 11:20 Suresh Bishnoi: *Descriptor-Based and Chemistry-Agnostic Machine Learning Frameworks for Property Prediction and Discovery of Glassy Materials*
- 11:35 Martin Andersson: *A microkinetic model for describing the molecular scale mechanisms that enhance aluminosilicate glass dissolution*

Symposium 1 (room: Tivoli og Vesterbros Torv)

Session chair: Seong H. Kim (assistant: Elsebeth J. Pedersen)

- 09:45 Theany To: *Fracture toughness of oxynitride glasses*
- 10:10 Haizheng Tao: *How to accurately determine the dynamic crack growth exponent for glass materials?*
- 10:35 Johan F. S. Christensen: *In situ mapping of indentation-induced densification and cracking in vitreous silica by nanofocus X-ray scattering*
- 10:50 Anders M. Schade: *Impact testing of screen protectors for mobile devices*
- 11:05 Dominique de Ligny: *Understanding local stress and structural modifications in glass using luminescence of Rare Earth Element and vibrational spectroscopy*
- 11:30 Stefano Marchesin: *Photo-induced structural dynamics in Ge-Se glasses: a comparative study in the X-ray and visible light range*

Lunch break

12:00 - 13:15

Symposium 3 (room: auditorium)

Session chair: Félix Q. Martínez (assistant: Sidsel M. Johansen)

- 13:15 Mette Solvang: *The role of ROCKWOOL stone wool production technologies and products in the green transition*
- 13:40 Denis Okhrimenko: *Development of in vitro biosolubility test for assessing stone wool fiber biopersistence*
- 14:05 Peter G. Jensen: *Improving high-temperature stability of stone wool fibres by optimizing crystallisation*
- 14:20 Susan Stipp: *Aluminosilicate glasses, weathering and solving the CO₂ challenge*

Symposium 5 (room: Enghave Plads og Kødbyen)

Session chair: Stephen Elliott (assistant: Søren C. J. Hansen)

- 13:15 [Jincheng Du](#): *Structures and structure-property relations of phosphate glasses: insights from atomistic simulations*
- 13:40 [Shingo Urata](#): *Cooling rate effects on CTE of sodium alkaline-earth aluminosilicate glasses*
- 14:05 [David L. Christensen](#): *Predicting Failure Regions in Sodium Silicate Glasses From its Initial Structure*
- 14:20 [Alfonso Pedone](#): *Unraveling the Mixed Glass Former Effect in Sodium Thiophosphate Glass Electrolytes: A Molecular Dynamics Perspective*

Symposium 1 (room: Tivoli og Vesterbros Torv)

Session chair: Steve W. Martin (assistant: Xiaoyi Xu)

- 13:15 [Doris Möncke](#): *Invert glasses of high optical basicity*
- 13:40 [Louis-Martin Poitras](#): *Insights into the Structure-Property Relationships and Conduction Mechanisms in Glassy Sulfide Electrolytes*
- 13:55 [Louisiane Verger](#): *New sodium-conducting glass compositions obtained by mechanochemistry: synthesis, structure, and properties*
- 14:10 [Xiaoyi Xu](#): *Role of organic linkers in controlling the deformation and fracture behavior of cyano-functionalized zeolitic imidazolate frameworks*

Coffee break and poster session

14:45 - 15:15

Symposium 3 (room: auditorium)

Session chair: Ashutosh Goel (assistant: Anders M. Schade)

- 15:15 [Alexandra Beltrami](#): *Surface evolution of alkaline silicate materials under ambient conditions*
- 15:30 [Santanu Mondal](#): *Selective leaching of stone wool at high pH by small organic molecules*
- 15:45 [Shuijiang Liu](#): *Surface crystallization of phosphate glass containing CuO and coloring on a float glass*

Symposium 5 (room: Enghave Plads og Kødbyen)

Session chair: Alfonso Pedone (assistant: Suresh Bishnoi)

- 15:15 Tao Du: *Atomistic Insights into Structure and Dissolution Behaviors of Metal-Organic Framework Glasses for Battery Applications*
- 15:40 Louis-Martin Poitras: *Establishment of Generalized Empirical Force Fields for Sulfide Glasses and Crystals Used as Superionic Electrolytes in All-Solid-State Batteries*

Symposium 1 (room: Tivoli og Vesterbros Torv)

Session chair: Søren S. Sørensen (assistant: Yong Li)

- 15:15 Yingbo Zhao: *Reticulating node-linker-strut chemical spaces for metal-organic network-forming glasses by synergistically promoting configurational degree of freedoms*
- 15:40 Minhyuk Kim: *Hybrid Glass Formation in Coordination Polymers via Aliphatic Chain Dynamics*
- 15:55 Meihua Qin: *Generic Vitrification of Prototype Metal-Organic Frameworks Linked by Rigid Dicarboxylate Linkers*

Abstracts - Monday June 15

Plenary session

Unraveling the origin of non-Zachariasen glasses

Matthias Wuttig, RWTH Aachen University, Germany

Almost one hundred years ago, W.H. Zachariasen wrote a seminal paper, in which he discussed the atomic arrangement in oxide glasses. He argued that oxide glasses like SiO_2 would have the same short-range order as the corresponding crystalline state, but lacked long range order. He postulated that the similarity in atomic arrangement would be a consequence of identical forces (we would now say: chemical bonds) between the atoms in both phases. Interestingly, phase change materials do not follow this conjecture, i.e., they form non-Zachariasen glasses. The difference of the short-range order between glass and crystal in these chalcogenides gives raise to significant differences in their property portfolio, such as the opto-electronic properties. These differences provide a vast range of application opportunities from rewriteable optical data storage, to active metasurfaces, non-volatile memories and neuromorphic computing. Hence, there are both scientific and technological reasons to unravel the origin of the non-Zachariasen nature of these chalcogenide glasses. Here we show that these glasses indeed change their bonding significantly upon crystallization, in contrast to the behavior of Zachariasen glasses. This statement is based on theoretical data employing quantum-chemical bonding descriptors as well as experimental findings utilizing atom-probe tomography. Only those glasses, where the corresponding crystal falls into a narrow range of these bonding descriptors, show the unconventional behavior of non-Zachariasen glasses. The corresponding crystals show a peculiar combination of properties not found in metallic, covalent or ionic solids. This is indicative for a special bonding mechanism in these crystals, a conclusion supported by the unconventional bond rupture observed in atom probe tomography as well as the unique positioning in the quantum chemical bonding map. The corresponding bond, which has been coined metavalent, is characterized by the competition between localization and delocalization. Utilizing this map, we can devise design rules for crystallization and vitrification kinetics, control the crystalline nanostructures as well as the contrast of the corresponding optical properties.

Manipulation of spectroscopic properties of active ions in glass via local structure

Lili Hu, Shanghai Institute of Optics and Fine Mechanics, CAS, China

With the rapid development of artificial intelligence (AI) and sensing technologies, there is an increasing and urgent demand on broadband amplifying components and laser medium for new laser band. Active ion-doped glass fibers represent one of the most promising platforms for achieving high-power lasers and broadband optical amplification, particularly within communication bands. Clarifying the intrinsic relationship between the local atomic structure of active ions and their luminescent properties is essential for breakthrough improvements in performance. In this talk, we will present our recent progress in understanding how the local structure of glass influences the luminescence behaviors of active ions such as neodymium and bismuth ions. By employing advanced characterization techniques, including Spherical aberration correction scanning transmission electron microscope (STEM), synchrotron X-ray total scattering, nuclear magnetic resonance (NMR), and electron paramagnetic resonance (EPR), we systematically investigate the interplay between local structure, thermal history, and the resulting optical properties. Our findings indicate that not only short-range but also medium-range structure significantly affects the luminescent behaviors of these active ions in glasses. Some of typical laser and amplifying properties of active fibers based on glass research will be demonstrated.

Symposium 2: Glasses for photonic devices, lasers, data storage, and processing tools

High Peak Power Fiber Lasers

Shibin Jiang, AdValue Photonics Inc, USA

All-fiber monolithic laser sources are highly desirable for many applications due to their compact and robust form factor. Recent advances in fiber laser technology have made fiber-based components readily available. We present high-peak-power fiber lasers—specifically, single-frequency pulsed systems achieving millijoule-level pulse energies at wavelengths near 1 μm , 1.55 μm , and 2 μm —enabled by our proprietary highly doped single-mode fibers with large mode-field diameters.

Lead-Free Perovskite-Doped Glasses: Promising Materials for White Light Emission

Nilanjana Shasmal, Federal Institute for Materials Research and Testing (BAM), Berlin 12489, Germany

In recent years, all-inorganic perovskite quantum dots (QDs) have become a major focus of investigation because of their outstanding electronic and optical characteristics. These features include exceptionally narrow emission spectra, adjustable photoluminescence (PL), high photoluminescence quantum yields (PLQYs), and strong optical absorption. Consequently, perovskite QDs are regarded as highly competitive candidates for use in photoelectric technologies such as light-emitting diodes (LEDs), photovoltaic devices, photodetectors, lasers, and anti-counterfeiting systems. Currently, lead (Pb) based compositions hold the record of PL efficiency, however, their real-world deployment remains constrained by critical issues, particularly the toxicity associated with this metal and the limited stability of their broadband PL emission. Lead-containing compounds pose severe health hazards, impacting neurological, cardiovascular, and skeletal functions, and once absorbed it is notoriously difficult for the body to remove. To mitigate these risks, extensive efforts have been directed toward substituting Pb^{2+} with less hazardous metal ions, including Sn^{2+} , Cu^{2+} , Mn^{2+} , Ni^{2+} , Zn^{2+} , Sr^{2+} , and Ba^{2+} . Among these options, Sn^{2+} is viewed as the most viable replacement because its ionic radius closely matches that of Pb^{2+} . In this work, lead-free perovskite QDs were synthesized directly inside a borosilicate glass host via a simple one-step melt-quenching method. Notably, this study reports for the first time the successful incorporation of CsSnCl_3 perovskites into a borosilicate glass matrix using the conventional melt-quench technique, yielding bright white emission under UV excitation. White light emission from Pb-free perovskites embedded in glass is of particular technological relevance for lighting applications. The resulting QD–glass composite displays intense and ultrabroad emission from 300 to 900 nm, producing visible white light and demonstrating strong potential for future W-LED applications. Replacing Pb entirely with Sn resolves the key toxicity concern, while the glass-ceramic strategy preserves the chemical robustness and emission stability of the QDs and greatly improves their suitability for integration into practical devices.

Tunable dual-band photoluminescent CsPbBr_3 quantum dots in glass for light-emitting applications

He Shasha, Wuhan University of Technology, Wuhan, China

All-inorganic cesium lead halide perovskite nanocrystals (NCs) or quantum dots (QDs) have received extensive attention in recent years due to their excellent photoelectric properties and quantum confinement effects. By adjusting the halogen components ($X=\text{Cl}$, Br , I) and the size of quantum dots, CsPbX_3 can achieve continuous luminescence tuning covering the visible light region (400–700 nm). However, the mixed perovskite system obtained based on halogen

ion exchange generally has stability problems and is prone to halogen phase separation, which seriously restricts its application in practical devices such as lighting and display. In this work, we in-situ precipitated CsPbBr₃ perovskite QDs in glass by melt quenching and subsequent heat treatment. By precisely adjusting the heat treatment temperature and time, CsPbBr₃ QDs with different sizes were obtained without halogen exchange. Small-sized blue-emitting CsPbBr₃ QDs and large-sized green-emitting CsPbBr₃ NCs are mixed and embedded in the glass, exhibiting dual-band emission centered at 450 nm and 490 nm, with narrow full width at half maximums of 25 nm and 21 nm, respectively. The CsPbBr₃ QDs embedded glass shows excellent long-term stability, and its luminescent color and crystal structure do not change. Studying the broad spectrum of CsPbBr₃ QDs can be applied to light-emitting diodes (LEDs), photoelectric sensors, lasers and other fields.

Preparation and Application of Mid-infrared Fluoride Glass Fiber

Yiguang Jiang, Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Shanghai, China

Fluoride glass optical fibers have low infrared transmission loss (<0.01 dB/m@2-5 μ m), low maximum phonon energy (<550 cm⁻¹), and a high laser damage threshold (≥ 40 MW/cm²), enabling full-spectrum and non-absorptive transmission of mid-infrared lasers, making them the most promising laser power transmission and laser gain medium for laser surgical equipment and infrared spectroscopy. However, at present, due to issues such as low purity of fluoride raw materials, significant crystallization tendency in fluoride fiber preform glasses, and the difficulty in preparing low-loss fluoride optical fibers, the development and application of mid-infrared optical fiber technology has been severely limited. In 2018, our project team laid out the research and development work on fluoride optical fiber materials. The team conducted a comprehensive study along the entire chain of raw materials for fluoride glass, glass melting, core-cladding structure design, preform rod preparation, and fiber drawing, achieving initial low-loss and high-quality preparation of fluoride glass fibers. The study proposed a sublimation purification technology based on different sublimation temperatures of impurity elements in raw materials, deeply purifying fluoride raw materials, achieving oxygen ions ≤ 1 ppm and trace impurities ≤ 100 ppb, laying the material foundation for fluoride glass fiber preparation. Additionally, based on first-principles calculations, the crystallization mechanism of fluoride glass fiber preform was revealed. This elucidation provides theoretical guidance for inhibiting crystallization of fluoride glass, enabling crystallization-free, large-scale preparation of fluoride glass. Furthermore, plasma surface treatment technology effectively removes the surface active oxide layer on the preform rod, addressing technical challenges such as crystallization, fish scale patterns, and minor defects during the soft glass drawing process, achieving high-quality, low-loss preparation of fluoride optical fibers.

Based on the advancement of passive and active fluoride glass fiber fabrication techniques, novel fiber laser devices and systems have been developed in recent years. With the Er-doped fluorozirconate fiber, high-power power amplifier systems for mid-infrared continuous-wave tunable lasers and broadband femtosecond lasers have been developed. Using the Dy-doped fluorozirconate fiber, passive mode-locking generating sub-ps pulses beyond the wavelength of 3 μ m, paving ways for molecular fingerprinting and other novel applications. Ultimately, a variety of fluoride optical fibers were developed, achieving optimal loss of <0.05 dB/m in preparation and stable transmission of 3.7-4.8 μ m laser >10 W@20 kHz, 30 ns, laying the foundation for fiber materials in medical surgery.

Regulation of micro/nano-structures and photonic functionalities of glass

Dezhi Tan, Zhejiang University, China

The regulation of micro/nano-scale structures and photonic functions serves as a critical foundation for the development of novel glasses and their new applications. A new mechanism

for glass structure regulation has been proposed, involving ultrafast laser-induced nanoscale phase separation and ion exchange. This has led to the invention of three-dimensional micro/nano-phonic structures with broadly and continuously tunable photoluminescence, and the development of miniaturized light-emitting devices such as glass-based micro-LEDs. Furthermore, a novel approach has been advanced to reduce the threshold for structural regulation through glass network design, enabling low-energy and rapid modification of glass structures. This facilitated the construction of novel hierarchical heterogeneous structures, specifically nanocrystals@amorphous-nanoparticle@glass composites, within which continuous-wave excited random lasing emission was discovered. Additionally, a deep learning-driven optical field manipulation method was developed to enhance the precision and efficiency of glass structural regulation, enabling the fabrication of low-loss three-dimensional optical waveguides and photonic interconnects. Furthermore, a butt-coupled optical chip architecture has been introduced, along with an ultra-broadband, low-energy nonlinear optical modulation method. This method exhibits a ultrasmall threshold for nonlinear activation function that is an order of magnitude smaller than previously reported, enabling the construction of an optical neural network. The invention of the first glass optical chip capable of all-optical nonlinear operations has notably improved the accuracy of image recognition and classification in optical neural networks through its nonlinear activation functions.

Chalcogenide Glass Fibers and Their Optoelectronic Sensing Applications

Yanqing Fu, Ningbo University

Chalcogenide glass fibers, with their broad infrared transparency window, low phonon energy, high optical nonlinearity, and semiconducting properties, exhibit great potential in infrared photonics, nonlinear optics, optoelectronic sensing, and flexible electronics, serving as a key platform for next-generation integrated optoelectronic systems. This report will provide a detailed introduction to multifunctional sensing technologies, device fabrication, and sensing applications based on novel chalcogenide glasses.

Facile and Quantitative Determination of Glass Redox State

Alexis Duval, FSU Jena - Otto Schott Institute of Materials Research

The redox state of glasses is a critical determinant of their optical, luminescent, mechanical, thermal, and electrical properties. Yet, its precise determination remains challenging, as commonly employed techniques are hindered by significant limitations: (i) limited accessibility (XANES, Mössbauer spectroscopy), (ii) the need for extensive prior standardization (ESR, Raman spectroscopy), or (iii) the risk of altering the redox state during measurement (XPS, EXAFS). In this study, we introduce two quick, accessible, yet precise wet chemistry methods for this purpose, relying on simple apparatus and easy-to-use reagents. The experimental protocol is unified across the various redox couples. These methods were validated using analytical standards encompassing diverse chemistry (oxides, nitrides, fluorides), and subsequently applied to a broad spectrum of redox couples and glass chemical systems (including mixed anion systems). Results demonstrated strong agreement with established methodologies, even enabling the accurate determination of highly reducing (Eu^{2+}) or oxidizing (Tb^{4+}) ionic species typically present in trace amounts in glasses.

Rare-Earth doped Glasses for (bio)Photonic Systems

Laetitia Petit, Tampere University (Finland)

The rapid evolution of photonic technologies demands advanced materials with tailored optical properties, high thermal stability, and broad functional versatility. Rare-earth doped glasses have emerged as pivotal candidates in this domain, offering unique advantages for

applications in lasers, optical amplifiers, data storage, and integrated photonic circuits. This invited talk presents recent breakthroughs in the synthesis, characterization, and application of novel rare-earth doped glass systems engineered for next-generation photonic devices. We explore the development of multicomponent glass matrices—such as tellurite, phosphate, and germanate—designed to optimize rare-earth ion solubility and enhance spectroscopic performance. Emphasis is placed on the strategic incorporation of ions like Er^{3+} , Yb^{3+} and Tm^{3+} , to achieve broadband emission, and low phonon energy environments. The talk further highlights the integration of these glasses into photonic platforms, demonstrating their utility in laser sources. Particular attention is given to the interplay between glass composition, thermal stability, and optical gain characteristics, which are critical for device reliability and scalability. Emerging trends such as composites and glass-ceramics and 3D structuring are also addressed, showcasing the transformative potential of rare-earth doped glasses in future biophotonic ecosystems. This presentation aims to illuminate the path toward multifunctional photonic materials driven by rare-earth innovation.

From Structure to Function: RE-doped Fluoride-Phosphate Glasses for Advanced Optical Applications

Andrea S. S. de Camargo, Friedrich-Schiller University Jena (FSU); Federal Institute for Materials Research and Testing (BAM)

Fluoride-phosphate (FP) glasses combine the advantages of fluoride networks—low phonon energy and reduced hygroscopicity—with the chemical and mechanical stability of phosphate frameworks, making them excellent hosts for rare-earth (RE) ions. These properties enable many applications such as in infrared lasers, scintillators, and integrated photonic devices. The ability to design optimized glass compositions relies on a deeper understanding of structure–property relationships based on advanced spectroscopic techniques. Our research explores FP glasses within Al- In- and Ga-containing compositional systems where fluoride partially substitutes phosphate, creating a tailored environment for RE ions. This approach reduces non-radiative losses and improves luminescence efficiency. Structural characterization using NMR, EPR, and Raman spectroscopy, combined with photophysical analysis, reveals how local coordination influences optical performance. For example, increasing fluoride content and modifying network connectivity enhance RE–F bonding, leading to longer excited-state lifetimes and reduced vibronic coupling. When it comes to scintillation, In-based glasses doped with Ce^{3+} and Tb^{3+} exhibit strong blue and green radioluminescence under X-ray excitation, matching detector sensitivity ranges. Al-based glasses doped with Er^{3+} are very promising materials for near-infrared lasing and in Ga-based FP glasses femtosecond laser writing enables spatially controlled formation of silver nanoclusters, which act as sensitizers for Nd^{3+} , boosting near-infrared emission and opening pathways for integrated photonic circuits. This presentation highlights our recent works and offers perspectives for the continued development of multifunctional FP glasses.

Optical Fiber Preform Materials: Novel Approaches in Powder Doping for Versatile Fiber Architectures in Medical and Industrial Photonics

Lothar Wondraczek, University of Jena

Specialty optical fibers, including large mode area (LMA) and multi-core architectures, require high-purity, reproducible core materials with precisely engineered refractive index profiles, tailored co-doping ratios, and optimized thermal processability. Silica-based fiber preform materials are the preferred option for high-power fiber lasers, high-resolution fiber endoscopic imaging, and fiber-based distributed sensing. Traditional fabrication methods are confronted with challenges: MCVD has difficulties with high concentrations, while powder doping in combination with crucible melting often introduces impurities. This presentation reviews fabrication pathways integrating modified chemical vapor deposition (MCVD) and novel

powder doping techniques to achieve scalable production of core materials for fibers with tailored numerical apertures and nearly perfect step-like distribution of various codopants. Electron probe micro analysis, Raman, UV-Vis, and FTIR spectroscopy confirm structural integrity, reduced clustering, and low OH⁻ content. This integrated approach represents a versatile platform in fiber core manufacturing, balancing performance, scalability, and sustainability for next-generation photonic applications.

CaTa₂O₆/Al₂O₃ composite ceramics prepared via crystallization from CaO-Ta₂O₅-Al₂O₃ glasses for highly-sensitive luminescent temperature sensing

Chen Tian, Wuhan University of Technology

Fluorescence intensity ratio (FIR) methods relying on emission from two thermally coupled energy levels are promising for remote temperature sensing but suffer from a limited temperature range. Here, CaTa₂O₆/Al₂O₃ composite ceramics with distinct cationic sites for multiple dopants are reported via crystallization from CaO-Ta₂O₅-Al₂O₃ glass precursors, which are supposed to be an alternative to overcome the above-mentioned drawback in field of luminescent thermometry application. With a controlled heat-treatment by rising the temperature step by step, α-CaTa₂O₆ nanocrystals were precipitated in the glass matrix at first, then β-CaTa₂O₆ were formed through a polymorphic transformation, and finally triggered the crystallization in the residual glass phase enriched in Al₂O₃. In the obtained composite ceramics, a woven microstructure consisting of interconnecting β-CaTa₂O₆ and α-Al₂O₃ crystals were observed, in which the average grain size is 310 and 200 nm, respectively. As a proof-of-concept, Er³⁺ and Cr³⁺ ions are introduced into the composite ceramics as the dopants. The active composite ceramics showed intense characteristic fluorescence mainly contributing to the emission of Er³⁺ in β-CaTa₂O₆ and the emission of Cr³⁺ in α-Al₂O₃. By tuning the Cr³⁺ concentration, thermal quenching behavior can be finely modulated, leading to a high emission retention of 186% at 573 K under simultaneous excitation. By combining thermally coupled and non-thermally coupled radiative transitions, the ceramic achieves a high relative sensitivity of 3.28% K⁻¹ at 348 K, and maintains a relative sensitivity above 0.85% K⁻¹ over a broad temperature range from 298 to 573 K. This work presents an alternative approach for the synthesis of composite ceramics as the host materials for highly-sensitive luminescent thermometry in high temperature operating conditions.

NIR-II emitting Ni²⁺ activated glass-ceramics prepared via controlled crystallization from MTa₂O₅-Al₂O₃ (M=Ca, Sr or Ba) glasses

Jian Ruan, Wuhan University of Technology

Owing to the rapidly development of NIR spectroscopy technology for non-invasive inspection broadband NIR pc-LEDs have been developing for replacing traditional tungsten lamp for minimize the light source. The overall performance of NIR pc-LED is significantly dependent on the broadband NIR light emitting materials. Especially, Ni²⁺ ion with a 3d⁸ electronic configuration has currently received considerable interests because of its NIR-II fluorescence generally with a FWHM wider than 200 nm. Here, MTa₂O₆:Ni²⁺ (M=Ca, Sr or Ba) glass-ceramics where Ni²⁺ ions are supposed to occupy Ta sites are reported. They were developed via crystallization from MTa₂O₅-Al₂O₃ (M=Ca, Sr or Ba) glass precursors with a controlled heat-treatment by rising the temperature step by step. The glass-ceramics exhibits a broadband NIR-II emission around 1200nm with an optimal Ni²⁺ doping concentration of 1.0 ~1.5 mol% and a PLQY more than 48% under excitation at 980 nm. By codoping with Er³⁺ ions, a dual-band NIR emitting glass-ceramics was obtained with an improve PLQY more than 57% under excitation at 980 nm. Combining the photoluminescence properties and microstructure characteristics evolution in the glass-ceramics, the Ni²⁺ in distorted octahedral geometry was discussed toward high-efficiency NIR-II emitting. At last, an illumination for NIR-

IR light source application was presented by determining the ethanol concentration in aqueous solution based on their difference in the NIR absorption spectra profiles.

Te-based chalcogenide glasses for use as thermal-imaging lenses: Momentum and potential

Yong Gyu Choi, Korea Aerospace University

Thermal-imaging cameras are expected to be integrated with automobiles in the form of advanced driver assistance systems (ADAS). The mandatory regulations relevant to the autonomous emergency braking (AEB) are set to come into effect in the coming years. Here, it is worth mentioning that the use of thermal cameras under foggy and/or nighttime conditions better guarantee the proper operation of the AEB systems. This unique advantage of thermal cameras would be more competitive in the market when a critical issue for the LWIR-imaging optics components is resolved: Specifically, the SWaP-C (size, weight and power consumption-cost) criteria should be applied when manufacturing lens assemblies operating at the long-wave infrared (LWIR) spectral range. This implies that both lens materials and lens-forming processes should be compatible with mass production of the lens assemblies that are more compact, lightweight, energy-efficient and cost-effective. In order to enhance flexibility in optical design of the lens assemblies suitable for the VGA grade thermal images, for example, use of more than doublet lenses is required. To facilitate the optical design and the subsequent precision glass molding (PGM) process, it is required to secure LWIR-transmitting chalcogenide glasses with a wider range of refractive index and its dispersion in a more broadened LWIR Abbe diagram. Majority of the commercially available chalcogenide glasses belong to compositional systems of Ge-(Sb or As)-Se and As-Se, both of which occupy only a limited region in the present LWIR Abbe diagram. Te-based chalcogenide glasses are typically more refractive but less dispersive across the LWIR range than Se-based counterparts, so that the corresponding refractive (and optionally diffractive) lenses can be more compact and more compatible with the PGM process. In this presentation, some characteristic features of Te-containing chalcogenide glasses are to be delivered with a focus on their thermal-imaging lens applications.

Temperature-dependent optical functions of selected Ge-Sb-Se bulk chalcogenide glasses determined using spectroscopic ellipsometry

Petr Nemeč, University of Pardubice

The determination of temperature dependent optical functions (refractive index (n) and extinction coefficient (k) spectral dependencies) for 5 selected bulk chalcogenide glasses was conducted in broad wavelength range (0.3 - 15 μm) at the temperatures from room temperature up to glass transition temperature (with reserve) using spectroscopic ellipsometry. Temperature dependence of bandgap energy obtained from Tauc-Lorentz oscillator model applied to measured ellipsometry data together with temperature dependence of refractive index for selected wavelengths (1.55, 3.4, 7.0 and 10.6 μm) are presented together with thermo-optic coefficients dE_g/dT and dn/dT for these wavelengths. For reference samples (Ge₂₈Sb₁₂Se₆₀ and As₄₀Se₆₀ commercial compositions), the obtained values for room temperature (namely refractive index) agree with values provided by the manufacturer and there is also considerably good agreement of thermo-optic coefficient dn/dT . In addition, we report dependence of refractive index and extinction coefficient in broad spectral range for selected temperatures together with the value of dE_g/dT . Remaining three glasses (Ge₂₈Sb₆Se₆₆, Ge₁₉Sb₁₇Se₆₄ and Ge₁₂Sb₂₅Se₆₃) were selected from (GeSe₂)_{100-x}(Sb₂Se₃)_x pseudobinary system. Increase of the absolute value of the refractive index as well as increase of the value dn/dT (for wavelengths 1.55 and 10.6 μm) can be observed with increasing content of Sb₂Se₃. Reported results are important for the exploitation of (GeSe₂)_{100-x}(Sb₂Se₃)_x glasses and their thin films in sensing applications.

Chalcogenide photonic devices and application in complex refractive index sensing

Wei Zhang, Ningbo University

Chalcogenide glasses are widely recognized as ideal materials for sensing, integrated photonics, and all-optical signal processing due to their broad transparent window, high linear and nonlinear refractive indices, low two-photon absorption coefficient, and negligible free-carrier absorption. Here, we present high-quality chalcogenide micro photonic sensor devices based on $\text{Ge}_{28}\text{Sb}_{12}\text{Se}_{60}$. Building upon conventional microring resonators, we fabricated slot Bragg gratings and slot microring resonator sensors using electron-beam lithography and inductively coupled plasma etching. By confining the optical mode in the low-index slit region, these structures enhance the interaction between the mode and the analyte, thereby improving sensor sensitivity. The achieved chalcogenide waveguide devices feature a minimum feature size of 150 nm, making them easier to fabricate compared to silicon-based Bragg grating devices. Measurement results show that the slot microring resonator exhibits a quality factor of 1×10^4 , a sensitivity of 471 nm/RIU, and an intrinsic detection limit of 3.3×10^{-4} RIU. Furthermore, beyond the real part of the refractive index, we simultaneously analyzed the effect of variations in the imaginary part of the complex refractive index on the resonant peaks of the transmission spectrum of the chalcogenide microring resonator. This enabled sensing of ternary mixed solutions. Experiments using ternary mixtures of water, heavy water, and methanol at different concentrations for complex refractive index sensing demonstrated a real-part sensitivity of 138 nm/RIU and an imaginary-part sensitivity of 341 nm/RIU. The above work lays a foundation for label-free multi-component sensing in biochemical and environmental monitoring applications.

Symposium 4: New non-oxide glasses, hybrid glasses and phase-change materials

Molecular doping into the metal-organic framework glasses for functional materials

Satoshi Horike, Kyoto University

Metal-organic framework (MOF) and coordination polymer (CP) glasses constructed from metals and organic ligands exhibit melting points in the 100–600 °C range, and their melts exhibit diverse chemical affinities. By exploiting these characteristics, functional molecules can be doped with high dispersion into these glassy states. For example, doping MOF/CP glasses with metal complexes that exhibit carbon dioxide reduction activity or photoresponsive behavior enables the synthesis of hybrid catalysts and ion conductors with high moldability and optical transparency. Furthermore, it is possible to construct phase diagrams between inorganic matters and MOF/CPs, opening a pathway for the exploration of novel inorganic–MOF hybrid functional materials.

Designing Vitrifiable Metal–Organic Frameworks through Coordination and Molecular Dynamics

Hoi Ri Moon, Ewha Womans University

Transforming metal–organic frameworks (MOFs) and coordination polymers (CPs) into amorphous or glassy states opens a new frontier that merges crystalline precision with the processability of soft matter. However, vitrification, especially in carboxylate-based systems with strong metal–ligand bonds, remains challenging. We reveal design strategies that couple coordination flexibility with molecular dynamics to achieve controllable vitrification. Mesophase-driven transitions in aliphatic carboxylate-based MOFs, ligand-rigidity tuning, and coordination-sphere perturbations in high-valent metal systems collectively demonstrate how molecular softness and entropy promote glass formation while preserving medium-range order.

These insights establish a unified framework for designing vitrifiable coordination materials that bridge crystalline, liquid, and glassy phases, expanding the structural and functional scope of reticular chemistry beyond crystallinity.

Chemical Approaches to Tuning the Structure and Properties of Hybrid Glasses

Sebastian Henke, TU Dortmund

Metal-organic framework (MOF) glasses can be processed in the supercooled liquid (SCL) state at elevated temperatures, enabling the fabrication of shapeable microporous materials for applications in phase-change memory, ion conduction, membranes, and (non-linear) optics. Unlike crystalline MOFs, whose structure and topology are typically fixed by precise composition, MOF glasses permit structural and functional tuning by the addition of so-called modifiers. In this approach, additives are introduced into the SCL to adjust coordination network connectivity and properties beyond the chemical and geometric constraints imposed by the crystalline frameworks. The SCL state provides flexible coordination environments, dynamic porosity, and the absence of long-range topological order, enabling chemical reactions inaccessible in the crystalline MOF solid. We show that incorporating organic, metal-organic, or inorganic modifiers into MOF liquids enables ligand incorporation, linker exchange, and salt dissolution directly in the melt. These liquid-phase modification pathways systematically tune the glass transition temperature, network topology, melt viscosity, and micro-/mesoporosity of the quenched glass. Controlled alteration of the metal coordination sphere via chelating co-ligands further enables adjustment of metal-centered properties, such as redox behavior and catalytic activity. Moreover, certain modifiers act as fluxes that allow vitrification of otherwise non-meltable MOFs, thereby expanding the accessible compositional and functional space. Overall, non-stoichiometric modification of MOF liquids provides a versatile and powerful strategy – analogous to modifier chemistry in oxide glasses and additive approaches in polymer processing – for the targeted tuning of structure and function in MOF glasses.

Iron-based zeolitic imidazolate framework glasses and beyond: from multi-structural phase transitions to direct synthesis

Guillermo Mínguez Espallargas, ICMol - University of Valencia

Metal-Organic Frameworks (MOFs) are a family of porous crystalline materials formed by organic ligands and metal ions (or clusters). A subfamily within MOFs is that of zeolitic imidazolate frameworks (ZIFs). Recently, this family has shown to be able to reach a liquid state prior to material decomposition which, upon cooling, vitrifies.[1] This glassy materials retain the basic metal-ligand connectivity of crystalline MOFs, which connects their mechanical properties to their starting chemical composition.[2] So far only a handful of ZIFs capable of reaching the liquid phase have been reported, including ZIF-4, ZIF-62 (Zn and Co) and ZIF-76.[3] Here we will present the preparation of the first Fe-ZIF glass, denoted ag-MUV-24, which is obtained via a three-step structural rearrangement from the known coordination polymer $[\text{Fe}_3(\text{im})_6(\text{Him})_2]$. [4] The melting temperature for $\text{Fe}(\text{im})_2$ is significantly below the melting temperature of the Zn analogue, thus potentially improving the applicability of the material. We will also show the possibility to incorporate other metal centres, such as Mn,[5] or even more than one metal in the same glass.[6] Finally, we will present a direct synthesis method for preparing a family of MOF glasses without relying on a meltable crystalline precursor, denoted dg-MUV-29.[7] This approach yields high-purity iron(II) MOF glasses while circumventing the oxidation and partial degradation typically associated with the conventional melt-quenching process. The absence of magnetic impurities enables us to investigate the intrinsic magnetic properties of the MOF glass, demonstrating that these materials serve as excellent model systems for topologically disordered amorphous antiferromagnets.

Furthermore, we highlight the functional benefits of direct-glass synthesis by fabricating free-standing glassy MOF films and incorporating them into optoelectronic devices.

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Taking a Magnifying Glance Through the MOF-Glass

Alexander Knebel, Friedrich Schiller University Jena

Metal-Organic Frameworks (MOFs) are a class of highly porous, crystalline materials, whose defined pore structure and versatile reticular chemistry are their characteristic features and have led to the Nobel Prize in Chemistry in 2025. In 2015, T.D. Benett and co-workers described the phenomenon of the glass transition of MOFs and their thermal amorphization and melt-quenching for the first time. By x-ray total scattering they demonstrated that the short-range order and network structure remained preserved in the resulting material. We studied the zeolitic imidazolate framework 62 (ZIF-62), as one of the best-known MOF-glass formers and its amorphous glass (agZIF-62) on changes of the porosity structure upon melt-processing. Millimetre-sized ZIF-62 single crystals were in-situ molten in a microscope heating stage, while kinetic gas uptake was probed in cm-scale melt-quenched agZIF-62 shards by in-situ IR-microscopy. We could elucidate the changes to the MOF-glass upon melting and when pressing the melt and quantify diffusion coefficients from kinetic gas uptake studies. Through this knowledge we were finally able to employ these glass in technical applications. We synthesize large, optical quality agZIF-62 by a re-melting and imprinting methodology to generate stimuli-responsive agZIF-62 microlenses. These photonic elements change their optical path length and thereby the refractive index when guest molecules are entering their empty pore space. Finally, by improving the melt-pressing of agZIF-62 by substrate matching of the coefficient of thermal expansion and ductility index we were able to generate stress and strain relaxed, large area MOF-glasses in a melt-pressing approach. From this it was possible to handle the agZIF-62 sheets and generate large area membranes with a thickness of 300 μm and a total size of 2.5 cm^2 . We employed these MOF-glass membranes for gas separation, with emphasis on sustainable technology for carbon capture processes.

Metal Organic Framework Glass Composites

Jingwei Hou, The University of Queensland

Metal-organic frameworks (MOFs) constitute a versatile class of porous materials with highly tunable structures and transport properties. While most MOF research has traditionally focused on their crystalline phases, our recent work has shifted towards exploring alternative structural states—most notably the glassy phase—which offers a distinctive combination of isotropy, enhanced stability, and exceptional processability. This unconventional form of MOFs has emerged as a promising materials platform for applications in molecular separation, mass transport, and related technologies. We have systematically investigated the thermal dynamics underlying MOF glass formation, with particular emphasis on the incorporation of silver ions and nanoparticles as composite-forming agents. These additives play a critical role in modulating the vitrification process, enabling the fabrication of robust and functional thin films suitable for membrane-based gas separation. The resulting MOF glass composites exhibit markedly enhanced gas transport performance for challenging separations, such as

light hydrocarbon mixtures, while simultaneously delivering improved thermal and mechanical stability. Beyond separation technologies, we have recently expanded the scope of MOF glass research into photocatalysis. By embedding photoactive components—including metal oxides and quantum dots—within the glassy MOF matrix, we have developed multifunctional composite materials capable of efficient light-driven reactions. These systems demonstrate strong potential for applications in solar fuel generation and environmental remediation, benefiting from the intrinsic robustness and tunability of the MOF glass network, as well as synergistic interfacial interactions between the host matrix and embedded functional species. Through these efforts, we aim to establish MOF glasses as a versatile and integrative platform for advanced membrane and catalytic technologies, combining efficient separation, long-term durability, and photocatalytic functionality. Collectively, our findings provide new insights into the rational design of next-generation materials with broad relevance to energy conversion, environmental sustainability, and chemical processing.

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Magnetism Evolution Induced by Structural Disorder in an Fe-Based Zeolitic Imidazolate Framework

Ang Qiao, Wuhan University of Technology

Modulating the degree of structural disorder in metal-organic frameworks (MOFs) offers a promising strategy for tuning their physical and chemical properties. Structural disorder in MOFs can be created by various means, e.g., heat-treatment or melting. Here we show that structural disorder can be induced in an iron-based zeolitic imidazolate framework (denoted as Fe-ZIF) by two methods, i.e., dynamic heating before melting and melt-quenching, respectively. On the one hand, by dynamically heating the Fe-ZIF to the temperature lower than its melting point, we observed a structural disorder primarily evolves at the medium- and long-range scales, while the short-range order remains largely preserved. And the degree of structure disorder can be tuned via changing the heating rate. Moreover, the magnetic measurements demonstrate that the sample with a higher degree of structural disorder exhibited a lower spin freezing temperature. On the other hand, we found that antiferromagnetic behavior in the crystalline Fe-ZIF transforms into weak ferromagnetism upon melt-quenching, i.e., during the transition to a structurally disordered glassy state. This magnetic transition is attributed to the enhanced exchange interactions between adjacent Fe II nodes, resulting from a reduction in the Fe II-Fe II correlation length from 6.2 Å in the crystalline phase to 6.0 Å in the glass. Thus, our work established the viable strategies for tailoring structural disorder in MOFs, thereby enabling precise modulation of their magnetic functions.

Continuous structure and property tuning of metal-organic framework glasses

Søren Strandskov Sørensen, Department of Chemistry and Bioscience, Aalborg University

Metal-organic frameworks (MOFs) have revolutionized materials science by their unique properties, e.g. as gas adsorbers and catalysts. However, they are usually restricted to powder form and “locked” to unique crystal structures within narrow composition ranges. This restricts the ability to tune their structure and properties, ultimately limiting their applicability. Recently, it was shown how some MOFs can melt and eventually form glassy phases free of grain boundaries – however still dependent on a stable molten phase of the parent MOF crystal.

Here, inspired by oxide glasses, we demonstrate a novel approach to creating stable MOF-based liquids that, upon cooling, transition into glasses with enhanced processability. This is achieved by mixing MOFs in the zeolitic imidazolate framework (ZIF) family with either water or halide salts (i.e., modifiers) in varying ZIF:modifier ratios. Depending on the ratio between MOF and modifier we show how it is possible to prepare glasses of otherwise unmeltable MOFs (e.g. ZIF-8) and continuously tune their structure and properties. Upon addition of halide salts to the ZIFs this allows lowering the glass transition of the ZIF glasses by $>200\text{ }^{\circ}\text{C}$ and creating centimetre-sized low-defect MOF glasses. Our modifier approach presents a platform for structure- and property-tuning in a wide composition range and may prove important for the expansion of the number of MOF glasses, optimization of their properties, and their applications in advanced materials engineering.

Ion Exchangeable Hybrid Glasses for Selective Mineral Harvesting from Seawater

Samraj Mollick, Aalborg University

The world's oceans hold immense reserves of strategically important minerals, but their low concentrations and chemically complex environments make selective extraction a persistent challenge. Conventional polymeric membranes and ion-exchange resins often fall short due to limited selectivity, slow transport kinetics, poor thermal stability, and short operational lifetimes. These constraints have hindered scalable, energy-efficient mineral recovery directly from seawater. In this work, we present a new class of ion-exchangeable hybrid glasses that address these limitations by merging the structural tunability of metal-organic framework (MOF) glasses with the chemical robustness of oxide-based glasses. By carefully blending ZIF-derived hybrid glasses with phosphate glasses and engineering chemical bonding at their interfaces, we create a mechanically stable, porous, liquid-like material designed for selective ion capture in highly saline environments. We demonstrate the performance of this platform using real seawater samples collected from geographically distinct sources, including the Red Sea (Saudi Arabia), Mediterranean Sea (Spain), and Baltic Sea (Denmark). In all cases, the hybrid glasses exhibit high selectivity and efficient recovery of magnesium as a mineral component. Leveraging the intrinsic moldability of these hybrid systems, we further fabricate a self-standing, durable membrane, overcoming the processing limitations of conventional MOF materials and enabling practical deployment for seawater softening. This study establishes hybrid glass membranes as a promising materials platform for scalable mineral extraction from seawater, offering a durable and energy-efficient route aligned with the growing demands of the blue economy.

Disorder-Enabled Isotropic Lithium Diffusion in Zeolitic Imidazolate Framework Glasses

Yong Li, Department of Chemistry and Bioscience, Aalborg University

All-solid-state lithium-ion batteries require solid electrolytes that combine rapid room-temperature ion transport with mechanical robustness and interfacial compatibility. Metal-organic framework glasses, particularly zeolitic imidazolate framework (ZIF) glasses, offer an attractive yet underexplored platform because they combine an amorphous, grain-boundary-free topology with chemically tunable frameworks. Here, we reveal how structural disorder unlocks fast lithium diffusion in ZIF glasses by using a machine learning interatomic potential to simulate Li-ion transport in crystalline and glassy ZIF-4 and ZIF-62. Vitrification reduces the Li⁺ migration activation energy from $\sim 0.35\text{ eV}$ in the crystals to 0.16 eV in both glasses, increasing the extrapolated room-temperature diffusion coefficient by more than one order of magnitude for ZIF-4 and by nearly sevenfold for ZIF-62. Analysis of non-Gaussian dynamics and van Hove correlation functions shows that crystalline ZIFs transport Li⁺ through rare, dynamically heterogeneous hopping events between well-defined cages, whereas ZIF glasses support more homogeneous, continuous, Fickian-like migration through a broadened

distribution of local environments. We further show that Li⁺ diffusion in crystalline ZIFs is strongly anisotropic, following $D_{yy} > D_{xx} > D_{zz}$, because ordered imidazolate and benzimidazolate ring orientations impose direction-specific barriers. Upon vitrification, these ring orientations become randomized, transforming anisotropic transport into isotropic or near-isotropic diffusion. These findings establish a direct structure-transport relationship between framework disorder, linker orientation, and Li⁺ mobility, identifying ZIF glasses as a promising design platform for room-temperature solid-state electrolytes.

Hierarchical microstructures in metallic glasses – are they real?

Robert Maass, Federal Institute of Materials Research and Testing (BAM)

Metallic glasses (MGs) are disordered solids that exhibit a range of outstanding mechanical, thermomechanical, and functional properties. Whilst being a promising class of structural materials, well-defined and exploitable structure-property relationships are still lacking. This offsets them strongly from their crystalline counterparts, for which length-scale based property determination has been key for decades. In recent years, both atomistic simulations and experiments have nurtured the view of heterogeneities that manifest themselves either as a structural partitioning into well-relaxed percolated network components and more frustrated domains in atomistic simulations (*Acta Mater* 209 (2021) 116771), or as spatially-resolved property fluctuations revealed across a variety of length scales (*Adv Func Mat* 28 (2018) 1800388). In this talk we discuss the emergence of such hierarchical and spatially resolved property fluctuations with an emphasis on length scales beyond 100 nm (*Appl Phys Lett* 106 (2015) 171907; *Mat & Des* 229 (2023) 111929). Such large length scales are hard to reconcile in a monolithic glass but may offer the perspective of experimentally easy-to-access length-scale based structure-property relationships. Whilst these large correlation lengths can be seen in both the plastic and elastic response, we focus here on high throughput nanoindentation mapping of extremely shallow elastic contacts. This approach is combined with advanced scanning-transmission electron microscopy in search of possible structural origins of the observed large correlation lengths. We demonstrate how these elastic microstructures are processing dependent (*Scripta Mater* 255 (2025) 116380) and that they seem to arise from internal atomic-scale strain fluctuations.

On the nature of the glass transition in metallic glasses studied via fast scanning calorimetry

Isabella Gallino, Tu-Berlin

Only recently, the development of fast differential scanning calorimetry (or chip-calorimetry) has allowed us to characterise in situ the glass transition response of metallic glasses during cooling from the liquid over a wider range of time scales employing scanning rates from 100 K/s up to 50,000 K/s. The generally accepted description is that the vitrification kinetics should exhibit the same temperature dependence as the relaxation time for the alpha-process. However, we have recently observed that vitrification at deep undercooling may occur with a milder temperature dependence than the alpha-relaxation [1-2]. The slower the system is cooled the more pronounced is the decoupling between these vitrification kinetics and the atomic mobility. As a consequence, vitrification can occur at fictive temperatures lower than those which would be obtained only accounting for the alpha-process. This apparent decoupling of the time scales for the vitrification kinetics from the time scales for the alpha-relaxation process is more pronounced at deep undercooling and for small sample sizes. This is of most importance because, it advocates a heterogeneity of cooperative atomic rearrangements, where faster mechanisms for atomic mobility that apparently are not contributing to the alpha-relaxation process, are maintaining the undercooled liquid system in (metastable) equilibrium and delay vitrification to lower temperatures.

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Design Strategies for Vitrification in Rare-Earth Carboxylate-Based Coordination Polymers

Yelim Lee, Ewha Womans University

Coordination polymers (CPs) exhibit exceptional structural tunability and hold great promise for a wide range of applications. However, their poor processability in crystalline or powder form limits industrial applications. To address this issue, transforming CPs into liquid or glassy phases has recently emerged as a promising approach. In particular, a direct vitrification (DV) pathway, the solid-to-glass transition without melting, has been widely employed. In this research, we present a new class of vitrifiable amorphous carboxylate-based CPs (aCeC4DC) composed of Ce^{3+} ions, an aliphatic carboxylate linker, adipate (C4DC, $-(\text{OOC})(\text{CH}_2)_4(\text{COO})-$), and a coordinating molecule, 1,4-diazabicyclo[2,2,2]octane (DABCO). We considered that the combination of the large ionic radius of the f-block cerium center and the flexible adipate linker with multiple coordination modes could facilitate the DV pathway. Leveraging these unique properties, we successfully obtained agCeC4DC (amorphous CeC4DC glass) by heating the aCeC4DC precursor to remove the coordinating DABCO, thereby inducing alternations in the coordination environment. The coordination sphere perturbation promoted vitrification, leading to the expansion of short-range order into medium-range order after vitrification. The vitrification process was characterized by differential scanning calorimetry, thermogravimetry analysis, and pair distribution function analysis.

Symposium 1: Fundamentals of glasses: formation, structure and physical properties

Infrared Light–Glass Interactions: Insights into Network Structure

Seong H Kim, Pennsylvania State University

Infrared (IR) spectroscopy provides a powerful lens into the three-dimensional connectivity of silicate glass networks. This talk begins with a brief review of how vibrational modes—particularly the Si–O–Si stretch and bend—encode structural descriptors such as bond length and angle distributions. We then revisit the long-standing interpretation of the $\sim 950\text{ cm}^{-1}$ shoulder, traditionally linked to non-bridging oxygens (NBOs). Recent nanoscale-FTIR and molecular dynamics studies reveal that this feature instead reflects network perturbations imposed by modifier ions and their relaxation during processes like Na \rightarrow H exchange, rather than isolated NBO vibrations. Building on these insights, we explore how IR spectral imaging techniques—such as scattering-type near-field optical microscopy and AFM-IR—enable imaging of subsurface structural changes. These methods uncover “invisible” damage from nearly elastic contacts and frictional slip, where bond-length elongation and angle distortion occur without topographic evidence, yet strongly influence light scattering, chemical durability and mechanical failure.

Hybrid Methods for Predicting Vibrational Properties of Glasses

Collin Wilkinson, Alfred University

Infrared optical properties are becoming critical for applications ranging from sustainability through defense applications. Despite the importance of infrared applications, predictions remain challenging due to the complexity of phonons in glasses. Here we present a hybrid

machine learning/molecular dynamics approach for accurately predicting the IR optical properties of common glasses. The predictions are compared with experiments and the utility of the methods are discussed.

Structure of Hydrated Borate Glasses

Elsebeth Juhl Pedersen, Department of Chemistry and Bioscience, Aalborg University

Structure of Hydrated Borate Glasses: Understanding the structural role of water in glasses is important for a range of phenomena, including the mechanical properties. For example, water can lead to stress corrosion, but more recent work has shown that steam treatment of some glass compositions can lead to improved crack initiation resistance, including in borate glasses. In this study, we therefore study the structure of $x\text{H}_2\text{O}(1-x)\text{B}_2\text{O}_3$ glasses with $x = 0.1, 0.2, 0.33,$ and 0.4 by melting B_2O_3 with varying amount of water in closed containers to incorporate water in the bulk borate glass structure. We characterize the structure through solid state NMR and x-ray and neutron scattering measurements. Particularly, we explore the hydrogen coordination environments by taking advantage of the different scattering lengths of the hydrogen isotopes. That is, we prepare glasses with either $1\text{H}, 2\text{H},$ or a combination thereof to obtain a null-scattering isotope composition of hydrogen, allowing the use of the isotope difference method to separate the hydrogen contributions from the borate network structure. We correlate the observed structural changes with the measured density and glass transition temperature.

Compositional Effect on Chemical Strengthening and Mechanical Properties of $\text{SiO}_2\text{-B}_2\text{O}_3\text{-Al}_2\text{O}_3\text{-Na}_2\text{O}$ Glass System for Enhanced Bending Resistance

Jinwook Jang, Department of Advanced Materials Engineering, Kongju National University, Republic of Korea

Sodium alumino-silicate (SAS) glasses are widely used as cover glass materials for mobile displays due to their excellent thermal stability, mechanical properties, and suitability for chemical strengthening. With the rapid development of foldable display technologies, however, ultra-thin glass (UTG) with thicknesses below $50\ \mu\text{m}$ has been employed but suffered from its vulnerability to impact damage, and crease formation along the folding axis causing a critical reliability issue. Improving crack resistance under repeated folding is therefore essential, which can be achieved by reducing the Young's modulus (E) and/or increasing the compressive stress (CS) introduced via chemical strengthening. Previous studies have shown that optimal ion-exchange behavior in SAS glasses is obtained when the $\text{Al}_2\text{O}_3/\text{Na}_2\text{O}$ molar ratio is unity, and that the addition of B_2O_3 effectively lowers the Young's modulus by modifying the glass network. Despite these findings, systematic studies on glass compositions that simultaneously achieve both a reduced Young's modulus and enhanced compressive stress after chemical strengthening are still limited, and the associated structure-property relationships have not been fully understood. In this work, a series of $\text{SiO}_2\text{-B}_2\text{O}_3\text{-Al}_2\text{O}_3\text{-Na}_2\text{O}$ glasses with a fixed $\text{Al}_2\text{O}_3/\text{Na}_2\text{O}$ molar ratio of 1 were prepared to investigate the effects of composition on mechanical properties and chemical strengthening behavior. The experiments were divided into two compositional series. In the first series, B_2O_3 was replaced by $(\text{Al}_2\text{O}_3 + \text{Na}_2\text{O})$ with the fixed SiO_2 content. While the second series, replaced SiO_2 with $(\text{Al}_2\text{O}_3 + \text{Na}_2\text{O})$ fixing B_2O_3 content. Glass samples were fabricated using a conventional melt-quenching method and their thermal and mechanical properties were examined. Young's modulus, Vickers hardness and the compressive stress and depth of layer after chemical strengthening were monitored. Structural changes induced by compositional variations and their relationships with mechanical properties were discussed with Raman spectroscopy, solid-state nuclear magnetic resonance, and X-ray photoelectron spectroscopy.

Correlating structural relaxation and fracture toughness in aluminoborosilicate glasses

Sidsel Mulvad Johansen, Department of Chemistry and Bioscience, Aalborg University

One of the biggest drawbacks of oxide glasses is their brittleness. This limits the scope of their applications and the need for thicker glass products. In the pursuit of developing more fracture resistant glasses, understanding the resistance to crack propagation, i.e. the fracture toughness, is paramount. Currently, it is not yet fully understood what structural features and energy dissipation mechanisms can improve the fracture toughness of oxide glasses. In this study, we investigate the fracture toughness of various calcium aluminoborosilicate glasses utilizing the Single-Edge Precracked Beam method. We also measure the α -, β - and γ -relaxation modes using Dynamic Mechanical Analysis. The activation energies for each type of relaxation are calculated, as the activation energy for the γ -relaxation has previously shown an inverse correlation with the fracture toughness of alkali aluminosilicate glasses. This study seeks to investigate if the same correlation applies to other families of oxide glasses, including if other relaxation modes should be considered.

Effect of B₂O₃ substitution for Al₂O₃ on crystallization behavior, microstructure, and mechanical properties of forsterite-based glass-ceramics

Liu Wei, State Key Laboratory of Advanced Glass Materials, Wuhan University of Technology

Glass-ceramics (GCs) with high mechanical performance are in growing demand for a wide range of applications, including aerospace, electronics, and biomedical fields. Compared with other systems, GCs based on the MgO-Al₂O₃-SiO₂ (MAS) system exhibit excellent mechanical properties. The crystallization of forsterite (Mg₂SiO₄) in glass significantly enhances its mechanical properties, including a high elastic modulus (~185 GPa for bulk Mg₂SiO₄), fracture toughness (4.9 MPa·m^{1/2}), and Vickers hardness (10.8 GPa). This study investigates the effects of B₂O₃ substitution for Al₂O₃ on the crystallization behavior, microstructure, and mechanical properties of GCs in the MgO-Al₂O₃-SiO₂ system. Upon heat-treatment, Mg₂SiO₄ crystallizes, though its content decreases with higher B₂O₃ levels, accompanied by increased crystal size and clustering. Spectroscopic and microscopic analyses (XRD, Raman, NMR, XPS, TEM) confirm that Ti³⁺ incorporates into the Mg₂ site of Mg₂SiO₄, while B³⁺ partially substitutes for Si⁴⁺. The fracture toughness of GCs initially decreases due to reduced crystallinity, but recovers at higher B₂O₃ contents owing to combined effects of larger crystal size and enhanced [BO₃] content. These findings provide insights into the role of B₂O₃ in tailoring the mechanical performance of Mg₂SiO₄-based GCs through controlled structural and microstructural evolution.

Indentation Deformation Mechanisms of Intermediate Calcium Aluminoborosilicate Glasses

Sourav Sahoo, Aalborg University

Oxide glasses are ubiquitous due to their excellent optical and chemical merits, but their poor fracture resistance limits their widespread use as structural components. Surface damage, such as indents and cracks inflicted by external rigid contacts, significantly deteriorates the practical strength of a glass product, and resistance to such damage is therefore a critical measure of its durability. Certain intermediate glass compositions, falling between the extremes of normal (shear-dominant) and anomalous (densification-dominant) glasses, are reported to possess higher indentation cracking thresholds; however, a detailed understanding of the underlying intermediate deformation mechanisms is still lacking. To this end, this study systematically investigates the indentation deformation behavior of a family of intermediate calcium aluminoborosilicate glasses and highlights the compositional dependence of micro-

hardness and crack resistance. Furthermore, the densification-to-shear proportion in the total deformed volume is quantified across multiple tip angles via sub-T_g annealing recovery, enabling characterization of the deformation evolution relative to normal and anomalous glasses. Finally, a careful inspection of the cross-sectional subsurface topography is carried out using atomic force microscopy to detect localized structural fingerprints of shear flow. Overall, this study elucidates the compositional dependence of intermediate glass deformation mechanisms and provides fresh insights into deformation pathways contributing to their improved mechanical response.

Experimental test of the isomorph theory: a step towards understanding glass-forming liquids

Kristine Niss, Roskilde University

When a liquid is cooled or compressed into a glass, its dynamics slows down dramatically—changing by many orders of magnitude. This change in relaxation dynamics is accompanied by subtle structural evolution. Isomorph theory predicts that all structural features and dynamics stay invariant along the same lines in the phase diagram; these lines are referred to as isomorphs. The theory works well for simple LJ-type systems in molecular dynamics (MD) simulations, but the question has been to which extend it is relevant for real experimental molecular systems. For more than a decade we have worked on developing and performing experimental tests of the isomorph theory. To probe the dynamics, we combine dielectric spectroscopy and quasielastic neutron scattering, accessing time scales from picoseconds to kiloseconds. This is combined structural studies by X-ray scattering and supported by MD-simulations on realistic molecular-models. Combining all these techniques we have tested a number of different isomorph predictions and established strong evidence that isomorph theory holds for van der Waals bonded liquids and gives some level of insight to ionic liquids and hydrogen bonding liquids as well. The implication is that any general theoretical description of viscous slowing down and the glass transition must be compatible with the framework provided by isomorph theory. Isomorph theory does not explain the glass transition but simplifies the problem by reducing the thermodynamic phase diagram from 2 dimensions to 1 dimension.

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Critical roles of activation entropy in relaxation and glass transition

Jun-Qiang Wang, Ningbo Institute of Materials Technology and Engineering, CAS

As the typical nonequilibrium characteristics, the physical origin of glass transition and relaxation kinetics are universal for different types of glasses. They have attracted broad interests but remain the most mysterious phenomena in condensed matter physics. In this talk, I will introduce our recent adventure in studying the nonequilibrium thermodynamics of glasses. It is found that both the activation free energy (G^*) determines T_g , while the activation entropy (S^*) determines m , where R is the gas constant. Based on the Boltzmann definition of entropy, the activation entropy is an indication of the number of the degeneracy of the evolution paths, which determines the fragility. It is also found that the nano-confined, low-dimension or high-pressured glasses exhibit much smaller S^* . It is interesting that the Kovacs memory effect in glasses appears only when the second-annealing process has a large S^* . A large value of S^* is a key requirement for observation of the memory effect and this may provide a useful perspective for understanding the memory effect in both thermal and athermal systems.

Broadband Shear Mechanical Measurements on Glass-forming Materials

Tina Hecksher, Roskilde University

Mechanical properties of glass-forming materials are central both for the fundamental questions in glass science and for applications. In the Glass & Time group, we have developed a broadband technique, the so-called Piezo-electric Shear Gauge (PSG), which can measure the dynamic shear modulus over a wide frequency span reaching up to 70 kHz [1-3]. The technique is optimized for relatively large moduli in the range 1 Mpa to 10 GPa and is thus ideal for measuring glass-forming materials near their glass transition temperature. Here, we explore the two hallmark dynamic features of supercooled liquids: non-exponential relaxation and non-Arrhenius temperature dependence of the relaxation time by in different types of glass-forming materials. We characterize the spectral shapes as well as multiple relaxation processes in the mechanical spectra and compare to other techniques [4-8].

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Structure determination in molecular amorphous solids with nonlinear optical properties

Hanna M. Wenzel, Philipps-University Marburg, Germany and Shimane University, Japan

Light-emitting diodes (LED) are highly energy efficient light sources. Light emission takes place in all directions in mainly the visible spectrum without heat loss in the infrared. [1] Recently, alternative light sources with highly directional irradiation properties have been found. These organotetrel chalcogenide clusters show extreme nonlinear optical properties by irradiation from a continuous-wave laser diode. If the compound consists of an amorphous matrix, a broad band emission in the visible region is seen. This effect is known as white-light generation (WLG). If the sample is crystalline, second-harmonic generation (SHG) takes place. [2,3] More specific, clusters with a general formula of $((RX)_4Y_6)$ show these characteristics, where R is an organic substituent, X is a group 14 element (Si or Sn) and Y is a group 16 element (S or Se). Depending on the organic substituent and X and Y, the resulting nonlinear optical effect is either SHG, e.g. $((NpSn)_4S_6)$ or WLG such as in $((PhSn)_4Se_6)$. [3-6] We performed molecular Reverse Monte Carlo modelling of the $((R_nSn)_4Y_6)$ clusters by fitting X-ray diffraction and extended X-ray Absorption Fine Structure (EXAFS) data simultaneously. Large distortions are present in the intramolecular structure of Ph- and Cp-substituted clusters. This is suspected to suppress crystallisation. [7] Results of the molecular Reverse Monte Carlo modelling as well as the inter- and intramolecular arrangements of the clusters will be presented.

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Pre-Existing Bicontinuous Structures in Oxyfluoride Glass Melts and Their Role in Ultrafast Nucleation Revealed by Chromatic Topological and Coarse-Grained Analyses
Kenji Shinozaki, National Institute of Advanced Industrial Science and Technology (AIST)

Understanding the mechanism of hierarchical structural ordering during glass formation is essential for elucidating the spontaneous nanocrystallization observed in oxyfluoride glasses. In this study, we investigate the structural evolution of $\text{BaF}_2\text{-ZnO-B}_2\text{O}_3$ oxyfluoride glass, which exhibits rapid nucleation and nanocrystallization even under press quenching, using classical molecular dynamics simulations combined with chromatic topological data analysis (chromatic TDA) and coarse-grained composition analysis. We demonstrate that a bicontinuous domain structure already exists in the high-temperature melt, at temperatures far above the melting point. This characteristic morphology is preserved during cooling with little geometrical evolution, thereby ruling out classical spinodal phase separation. Notably, the characteristic length scale of the bicontinuous domains is already established in the melt and remains nearly constant over a wide temperature range, indicating that cooling does not drive domain coarsening but instead governs internal chemical evolution within geometrically constrained domains. Coordination analysis reveals pronounced bond selectivity. Ba-B and Ba-O coordination environments show minimal temperature dependence, indicating that the oxide network is structurally stabilized at an early stage. In contrast, Ba-F and Ba-Ba coordination numbers increase systematically upon cooling, reflecting selective stabilization and chemical purification within Ba-rich domains. This behavior is governed by enthalpic preferences consistent with the Hard and Soft Acids and Bases (HSAB) theory. Zn plays a crucial interfacial role in this process. Although Zn is intrinsically more stable in the B-rich phase, it partially occupies Ba-rich regions in the high-temperature melt. As cooling proceeds, Zn is progressively expelled from the cores of Ba-rich domains toward B-rich and interfacial regions, facilitating the selective development of Ba-F-rich structures while suppressing complete macroscopic phase separation. Importantly, coarse-grained analysis reveals that the pre-existing fluoride-rich domains in the melt already exceed the critical nucleus radius for BaF_2 crystallization, providing structurally favorable precursors for nucleation. As a result, nucleation is no longer limited by rare density or compositional fluctuations, enabling exceptionally fast nucleation upon cooling. These results demonstrate that cooling primarily induces chemically selective maturation within pre-existing bicontinuous domains rather than morphological growth, highlighting structural design in the melt as a key factor controlling nucleation kinetics.

Plasma melting $\text{Al}_2\text{O}_3\text{-RxOy}$ binary aluminate glass and transparent ceramics microspheres

Jihong Zhang, Wuhan University of Technology

High-strength aluminate microsphere materials have important applications for additive manufacturing, sealing, display, injection molding, and others. The fabrication of aluminate transparent ceramics and glass microspheres are still challenging due to their high melting temperatures. In this research, various binary aluminate microspheres were prepared using radio frequency plasma melting technique. The morphologies, structure evolutions, and mechanical performances were investigated. For $\text{Al}_2\text{O}_3\text{-CaO}$ microspheres, the average diameter is around 35 μm . The main crystal phases change from the combination of CaAl_4O_7 and $\text{Ca}_3\text{Al}_{10}\text{O}_{18}$, to $\text{Ca}_3\text{Al}_{10}\text{O}_{18}$ and CaAl_2O_4 , then to CaAl_2O_4 and CaAl_4O_7 with decreasing $\text{Al}_2\text{O}_3/\text{CaO}$ ratio. While glass microspheres were formed with 36 Al_2O_3 -64 CaO component. The microspheres exhibit maximum 12.73 GPa microhardness and 133.16 GPa Young's modulus, from mixed crystal phases evolutions and decreasing 9.25 GPa microhardness and 96.64 Young's modulus for 36 Al_2O_3 -64 CaO from amorphization. $\text{Al}_2\text{O}_3\text{-ZrO}_2$ binary microsphere present eutectic characteristics, containing $\alpha\text{-Al}_2\text{O}_3$, $t\text{-ZrO}_2$, $m\text{-ZrO}_2$ crystals, with maximum 23.21GPa microhardness, and 211.80GPa Young's modulus.

Moreover, other binary aluminate microspheres, such as Al_2O_3 - Y_2O_3 , Al_2O_3 - Gd_2O_3 , will be discussed.

Crystallization Mechanism of Fluorine-Oxygen Glasses – Elucidated by Solid-State NMR Spectroscopy

Jinjun Ren, Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences

Oxyfluoride glass-ceramics exhibit considerable potential for applications such as 3D displays, solar cells, and white-light illumination, primarily owing to their efficient up-conversion luminescence. The performance of these materials is fundamentally determined by the distribution of rare-earth ions between the glass and crystalline phases, which itself is governed by the crystallization mechanism of fluorine-containing phases. This presentation utilizes advanced solid-state nuclear magnetic resonance (NMR) spectroscopy to elucidate the atomic-scale structural evolution during heat-induced crystallization. By integrating structural insights from solid-state NMR, we systematically investigate the crystallization mechanism of fluorine species within the glass matrix and delineate the roles of rare-earth ions and other constituents at the atomic scale. Building on this mechanistic understanding, we explain how and why rare-earth ions distribute across phases, thereby establishing a foundational framework for the targeted optimization of these functional materials.

Growth of secondary phases on calcium aluminosilicate glass surfaces

Néstor Merino-Díez, Danmarks Tekniske Universitet (DTU)

Calcium aluminosilicate (CAS) glass provides a model system that can be used to explore the reactivity of natural amorphous materials originating from volcanic and metamorphic environments such as basaltic or impact glasses. It is also useful for understanding glass behaviour in general, for providing insight into the short and medium range order of glassy materials, predicting their long-term performance and stability and for contributing background for global geochemical process models, such as for weathering reactions. We investigated CAS glass surface reactivity in air, over a range of relative humidities, using analytical techniques with molecular scale resolution, mainly atomic force microscopy (AFM). We observed the growth of secondary phases on the glass surface, where form and abundance depend on humidity of the air in contact. These results are important for understanding how glass network forming (Si, Al) and modifying elements (Ca, Na, other cations) influence glass surface behaviour, which contributes to the design and application of sophisticated amorphous materials, particularly in environments where prolonged exposure to varying humidity is expected.

Abstracts - Tuesday June 16

Plenary session

Reinventing soft glasses and fibres through adding crystal particles, tuning fibre microstructure or processing in microgravity

Heike Eborndorff-Heidepriem, Adelaide University

This talk reviews the versatility in properties enabled by soft glasses and fibres through controlling glass composition, doping luminescent species (rare earth ions, crystal particles), using fabrication technologies enabling a diverse range of cross-sectional structures and processing in microgravity conditions. Examples are:

- tellurite and silicate glass fibres doped with diamond particles containing nitrogen vacancy centres for quantum-based magnetic field sensing
- tellurite glass fibres doped with Er:YAP microcrystals for proof-of-concept of new laser material concept
- tellurite glass doped with luminescent rare earth ions for temperature sensing and volumetric display
- variety of oxide glasses with in-situ grown gold and silver nanoparticles for plasmonics, glass art and tissue-mimicking phantoms
- impact of casting and extrusion methods on core/clad interface quality of soft glass fibres
- new microstructured fibre concepts through soft glass extrusion
- ZBLAN fluoride glass fibres drawn in microgravity for next generation fibre optics cables for conventional and quantum communication

Atomistic Understanding of Structure, Relaxation and Related Phenomena in Chalcogenide Glasses and Glass-Forming Liquids

Sabyasachi Sen, Department of Materials Science and Engineering, University of California, Davis, USA

Chalcogenide glasses are an important class of materials that are sulfides, selenides or tellurides, mainly of Ge, As, P and Si with minor concentrations of elements such as Ga, Sb, In and La, which have found wide ranging technological applications in the areas of infrared photonics, telecommunication, remote sensing, energy and memory storage. Compared to oxide glasses, the compositional flexibility of chalcogenides allows for excellent tuning of their various technologically relevant physical properties. This tunability arises from remarkable compositional evolution of the atomic structure of these glasses, which may range from linear chains to highly crosslinked networks all the way to zero-dimensional molecules and molecules embedded in a polymeric matrix. The attendant change in the connectivity of the network may be linked to rigidity percolation, and it markedly influences the temperature dependence of the configurational entropy and the rheological properties of the parent glass-forming liquids. Some of these liquids can also undergo pressure and temperature induced polyamorphic structural transformations e.g. from a low-density molecular liquid into a polymerized high-density liquid. In this talk I will present results of systematic investigations of these phenomena, obtained using a unique combination of state-of-the-art spectroscopic, thermodynamic and rheometric characterization techniques. These results are used to build a mechanistic understanding of how these phenomena are controlled by the connectivity and topology of the atomic structure, in a wide variety of chalcogenide glasses and liquids.

Symposium 2: Glasses for photonic devices, lasers, data storage, and processing tools

The R&D of the High Light Yield and High Density Glass Scintillator for High Energy Physics Detectors

Sen Qian, The Institute of the High Energy Physics, CAS

Scintillation materials can convert high-energy rays into visible light. Compared with crystal scintillator, the glass scintillator has many advantages, such as a simple preparation process, low cost and continuously adjustable components. Therefore, glass scintillator has long been conceived for application in the nuclear detection such as hadronic calorimeter. In 2021, the researchers in the Institute of High Energy Physics (IHEP) have set up the Large Area Glass Scintillator Collaboration (GS group) to study the new glass scintillator with high density and high light yield. Currently, a series of high density and high light yield scintillation glasses have been successfully developed. The density of Ce³⁺ doped borosilicate and silicate glasses exceed 6 g/cc with a light yield of 1000 ph/MeV. We have already studied the energy deposition of the best performance glass scintillator with different particles (cosmic ray muons, electrons, pions, protons, etc.); completed the radiation resistance of glass scintillator under proton beam and gamma irradiation, Finished the modeling of scintillating glass in GEANT4 for better consistent the simulation results with experimental data. The scintillating glass collaboration team will continue to develop scintillating glass for high-energy radiation detection applications.

Lead-free halide nanocrystals in glass: tailoring luminescence for advanced optoelectronic applications

Chao Liu, State Key Laboratory of Advanced Glass Materials (Wuhan); Silicate Materials Engineering Research Center, Wuhan University of Technology

Recent advances in glass-embedded nanocrystals with luminescent properties have enabled important potential applications in data storage, lasers, anti-counterfeiting, high-energy photon detection, and imaging. Among these, cesium lead halide perovskite nanocrystals embedded in glass have attracted considerable attention due to their composition-tunable band gap, defect tolerance, and high photoluminescence quantum yields. However, the presence of toxic lead in these materials has hindered their broader application. This presentation will review recent progress in the development of lead-free halide nanocrystals embedded in glass matrices. Through melt-quenching and controlled thermal treatment, we have achieved the in-situ formation and encapsulation of various lead-free nanocrystals, including cesium manganese halides, cesium alkaline-earth halides, and cesium rare-earth halides. The photoluminescence properties of these glass-embedded nanocrystals-such as emission wavelength, spectral linewidth, lifetime, and quantum yield-have been effectively tailored by adjusting their size, composition, and dopant ions. Furthermore, the chemical, thermal, and photostability of these materials have been systematically evaluated to assess their practicality for real-world applications. A detailed discussion on the structure-property relationships governing the photoluminescence behavior of these nanocrystals in glass will be provided. Finally, we will demonstrate their potential in emerging applications such as light-emitting diodes, X-ray detection, and imaging technologies.

Hybrid Glass Fiber and Its Optical Applications

Guoping Dong, Department of Inorganic Materials Science and Engineering, South China University of Technology

Combining the merits of the high efficient luminescence of nanocrystals and the excellent fiber-drawing ability of the glass matrix, transparent nanocrystal-doped glasses and fibers have

been considered as potential candidates for various optical applications. Our group designed the glass system based on glass genetic engineering prediction, and controlled the formation of low phonon energy nanocrystals in the glass matrix through external field induction. The high performance nanocrystal-doped glass fibers were fabricated by novel fiber-drawing method. Importantly, enhanced visible and infrared laser output is realized in nanocrystal-doped glass fibers, strongly manifesting that the obtained hybrid glass fiber is a promising gain material for fiber lasers. Furthermore, our works also expanded the potential applications of nanocrystal-doped glass and fiber in fields of amplifier, sensor, detecting, etc.

Ultrafast Laser 3D micro-nano Fabrication of Core Architectures for Glass-based Photonic Quantum Chips

Zhi Chen, Kunming University of Science and Technology

The development of silicon-based electronic circuits is limited by Moore's Law, which is full of challenge for manufacturing an electronic circuit with a unit size below 5 nm. Compared with electrons, photons provide more design degrees of freedom, including: phase, polarization, mode, orbital angular momentum, frequency, and etc., and photonic circuits using photons as carriers have unique advantages in the information storage, propagation, and processing, such as: ultra-large information capacity, Ultra-low energy consumption, and ultra-high operating speed. A complete photonic circuit is composed of thousands of micro-/nano-photonic integrated devices, and its performance is directly affected by the quality of the material and the device structure processed. In recent years, femtosecond laser manufacturing technique has been considered as a high efficient approach to fabricate micro-/nano- photonic integrated devices. However, there exists an issue that it is hard to precise control the manufacturing size, shape, spatial mode, and refractive index distribution of a photonic device by conventional femtosecond laser processing strategy, for a long time. In this presentation, we will focus on sharing our latest research progress in the fields of new optical waveguides devices based on femtosecond laser direct-writing with spatial resolution as high as 700 nm, nanophotonic structural devices approaching 10 nm, and looking forward to their potential applications in optical amplifiers, lasers, sensors, and beam manipulation.

Tellurite fibre fabrication with NV-containing diamond particles using an interface-based approach

Sachin Kumar, Adelaide University

Diamond containing nitrogen-vacancy (NV) centres are promising for magnetic field sensing via optical detection. Incorporating NV-diamond particles into optical fibres allows the guided modes of the fibre to be used for efficient excitation and collection of NV fluorescence, enabling remote and distributed sensing geometries. Tellurite glass is an attractive host for incorporating NV-diamond particles into optical fibres as it offers low processing temperatures and good fibre drawability, which is favourable for NV-diamond preservation. The high refractive index of 2.0 of tellurite glass reduces scattering by diamond particles with index ~ 2.4 . NV magnetometry sensitivity can be enhanced by exploiting external absorption or laser emission coinciding with NV energy levels. In this work, we investigate tellurite glass fibres with a core doped with NV-diamond particles and co-doped Yb₂O₃ to utilize interaction between the Yb³⁺ emission near 1042 nm and the infrared absorption of NV centres for ultimately achieving lasing-enhanced magnetometry in a fibre. The cladding is undoped using the composition of 75TeO₂–10Na₂O–15ZnO. Refractive index measurements of tellurite glass samples made from the Yb-free clad glass and an Yb-containing glass (77TeO₂-10Na₂O-12ZnO-1Yb₂O₃) confirmed that Yb₂O₃ doping reduces the refractive index as observed for other lanthanide-doped tellurite glasses. To compensate this, we increased the TeO₂ content in the core glass to 79TeO₂-10Na₂O-10ZnO-1Yb₂O₃ to obtain the target numerical aperture of NA ~ 0.1 . A key challenge for NV-diamond fibres is balancing NV fluorescence strength with

fibre loss caused by scattering from the diamond particles. To address this, two different spatial distributions of the diamond particles within the fibre core will be investigated: a ring-shaped distribution at a defined radial position within the core, similar to interface-doped fibres, and a volumetric distribution across the core. This will provide guidance on particle placement strategies for optimising NV-diamond doped tellurite fibres.

Perovskite nanocrystals in glass for high efficiency and ultra-high resolution dynamic holographic multicolor display

Chao Ruan, State Key Laboratory of Extreme Photonics and Instrumentation, College of Optical Science and Engineering, and School of Materials Science and Engineering, Zhejiang University, Hangzhou 310027, China

Incorporating all-inorganic lead halide perovskite nanocrystals (PNCs) into the glass matrix has been demonstrated to be an effective route to improve their environmental stability for long-term operation. Despite the significant improvements in the photoluminescence quantum yield (PLQY) of PNCs-glass composites in recent years, simultaneously achieving high luminance and high PLQY remains challenging. Herein, we report a strategy that employs fluoride ion doping to modify the three-dimensional glass network and lower the glass transition temperature (T_g), thereby optimizing the crystallization behavior of PNCs and achieving both high luminance and high PLQY across the full spectrum. Leveraging these high-performance composites, we constructed a dynamic holographic multicolor display system by integrated with a spatial light modulator (SLM), achieving a pixel density over 2×10^4 pixels per inch (PPI). The composites exhibit high transparency, which allows us to further propose a vertically stacked, multilayer full-color display architecture that overcomes the limitations of color filters in light-utilization efficiency and the bottlenecks of conventional planar sub-pixel layouts in terms of spatial utilization and resolution.

Infrared optics with gradient refractive index based on chalcogenide glasses

Xianghua Zhang, University of Rennes/CNRS

Chalcogenide glasses are now widely used as optical materials for thermal imaging. For an increasing number of applications, it is desirable to develop compact, lightweight and highly efficient imaging systems. One promising solution is the use of optical components with a graded refractive index (GRIN). To create such refractive index gradients, several research groups have proposed different approaches, including interdiffusion, controlled graded crystallization, and ionic exchange. Each of these methods presents specific advantages and limitations, which will be analyzed in this presentation. In this work, we have focused on the ion-exchange method and selected a stable glass composition from the $\text{GeSe}_2\text{-Ga}_2\text{Se}_3$ system. This composition exhibits a relatively high glass transition temperature, allowing it to withstand the highly corrosive conditions associated with ion-exchange processes. An appropriate amount of NaI was introduced into the base glass in order to provide a sufficient concentration of mobile Na^+ ions while maintaining adequate chemical durability. Na^+/K^+ ion exchange was first carried out by immersing the glass in a molten nitrate salt containing K^+ ions. Even under optimized conditions, achieving an ion-exchange depth greater than 2 mm proved difficult, requiring immersion times of up to 40 days. Under these conditions, the maximum refractive index change was typically limited to about 0.045. More recently, Na^+/Ag^+ ion exchange has been achieved using a quasi solid–solid process, developed to overcome the excessive corrosivity of Ag^+ -containing molten salts. Under optimized conditions, an exchange depth exceeding 6 mm can be obtained within approximately 30 hours. Moreover, the maximum refractive index change can exceed 0.1. These results demonstrate the strong potential of this approach for practical infrared GRIN optical applications.

Recent Advances in Chalcogenide Glasses and Acousto-Optic Devices: From Structure–Property Correlations to Low-Power, High-Performance Modulators

Shixun Dai, Ningbo University

Acousto-optic (AO) devices are key components in modern photonic systems, enabling rapid and efficient modulation, deflection, and signal processing over a broad spectral range. Chalcogenide glasses have attracted sustained interest as AO media owing to their high refractive indices, wide infrared transparency, and excellent compositional tunability. Nevertheless, their practical application has long been limited by intrinsic trade-offs among acousto-optic figure of merit (M_2), acoustic attenuation, thermo-optic coefficient, laser-induced damage threshold (LIDT), and mechanical stability. Since 2021, our research group has systematically investigated novel sulfur- and selenium-based chalcogenide glasses and their AO device applications. This invited review summarizes recent progress achieved through correlating glass composition, network structure, and AO performance, and through translating optimized materials into practical low-power AO devices. We first discuss structure–property relationships in representative chalcogenide glass systems, including As–S, As–S–Te, Ge–As–S, Ge–Sb–S, and Ge–Sb–Se glasses. Raman and compositional analyses reveal that the evolution of fundamental structural units—such as $[\text{AsS}_3]$ pyramids and $[\text{GeS}_4]/[\text{GeSe}_4]$ tetrahedra—plays a decisive role in controlling network connectivity, acoustic velocity, and energy dissipation, thereby governing the balance between high M_2 and low acoustic attenuation. To address toxicity and reliability concerns, arsenic-free chalcogenide systems, including Ge–Sb–S, Ge–Sb–Se, and Ge–Sn–Se–S glasses, are further developed. Through compositional substitution, graded S/Se interchange, and controlled nanocrystallization, simultaneous enhancement of AO efficiency, thermal stability, and LIDT is achieved. Finally, we demonstrate fiber-coupled AO modulators operating at 1.55 μm based on optimized chalcogenide glasses, exhibiting high diffraction efficiency, low radio-frequency drive power, fast response, and stable operation. These results establish a coherent framework linking glass structure, AO properties, and device performance, highlighting chalcogenide glasses as versatile platforms for next-generation high-performance AO applications.

Femtosecond laser writing of mid-infrared splitters in chalcogenide glasses

David Le Coq, University of Rennes

Chalcogenide glasses are promising materials for high-performance optics, particularly in the mid-infrared (MIR) range. Beyond their exceptional infrared transparency, they exhibit high photosensitivity to femtosecond lasers, enabling the inscription of optical integrated structures. Various writing techniques can be employed to modify the refractive index of the glasses. In this presentation, we will first focus on a point-by-point process, which allows precise control over both the refractive index modification and the dimensions of photowritten waveguides. The resulting structures exhibit low propagation losses and high coupling efficiency from free space, making them highly suitable for advanced MIR optics. This includes straight and curved waveguides, as well as couplers and Y-splitters. We will also discuss recent advancements, including a 1×6 splitter demonstrating a linear power distribution among the 6 channels, highlighting the potential of these materials for integrated photonic applications.

Chalcogenide Glass Thin Films as Functional Materials for Infrared Photonic Water Pollution Sensors

Virginie Nazabal, CNRS and University of Rennes

Chalcogenide materials are promising candidates for mid-infrared (MIR) integrated optical sensors dedicated to water quality monitoring. Their wide transparency range in the MIR, high refractive indices, and tunable compositions make them well suited for evanescent wave spectroscopy. This sensing approach is particularly relevant for the detection of organic

molecules in water, an important environmental challenge caused by industrial, agricultural, and pharmaceutical pollution. MIR spectroscopy enables direct access to the fundamental vibrational modes of chemical bonds, allowing selective and reliable identification of organic compounds. However, conventional MIR spectroscopic systems are often bulky, costly, and not adapted for in situ measurements. Integrated photonic sensors based on chalcogenide waveguides provide an effective alternative, offering compactness, robustness, and real-time operation. In this work, we develop a chalcogenide-based MIR sensing platform using arsenic-free GeSe₂ thin films. The films were deposited by RF magnetron sputtering, a scalable technique compatible with standard microfabrication processes. Deposition parameters were optimized to obtain uniform films with controlled thickness and low optical losses, suitable for planar waveguide fabrication and operation in aqueous environments. The chalcogenide thin films were characterized using atomic force microscopy, spectroscopic ellipsometry, and Fourier-transform infrared spectroscopy. The results demonstrate good thickness uniformity, low surface roughness, and propagation losses comparable to state-of-the-art MIR integrated devices. Taking advantage of the tunable optical properties of chalcogenide materials, the waveguide geometry was optimized to balance optical confinement and evanescent field penetration into water, maximizing interaction with dissolved organic analytes. To improve stability and selectivity in water, the waveguides were functionalized with a hydrophobic polymer coating. This layer reduces water infiltration and non-specific adsorption while maintaining transparency in the MIR range. The proposed platform provides a solid basis for compact and reliable chalcogenide-based MIR sensors for real-time, in situ water monitoring.

Non-conventional laser processing of glass

Félix Quintero Martínez, CINTECX, Universidade de Vigo, LaserON, 36310 Vigo, Spain

The development of lasers has been intrinsically linked to glass since the first laser was built in 1960. Glass has enabled key advancements, from early solid-state and gas lasers to the invention of optical fibers in 1970, which revolutionized laser applications. Fiber lasers, derived from doped optical fibers, offer high efficiency and versatility, representing a major leap in laser technology. Today lasers are used commercially for different glass processing applications such as marking or cutting. This paper explores non-conventional laser-based glass transformation processes such as Laser Spinning or Cofiblas, two innovative techniques to produce glass nanofibers with unique physicochemical properties. Both methods employ a high power laser capable of heating the precursor material from ambient temperature up to 2000 °C within milliseconds, combined with a supersonic gas jet which stretches and cools the high-temperature melt to ambient temperature in times of the same order of magnitude. In this way, both techniques produce glass nanofibers even from materials that are very prone to crystallization. Also explores laser-assisted additive manufacturing of glass. Using lasers as energy source for additive manufacturing of glass is an emerging field useful also for recycling glass wastes as those form pharmaceutical glass containers. The particular properties of lasers allow glass to be processed in ways that are completely different from conventional methods, thus transforming glass into three-dimensional pieces with tailor-made shapes or into nanofibers with extraordinary properties.

White-light emission in zeolitic imidazolate framework glasses

Zhencai Li, Aalborg University

Zeolitic imidazolate framework (ZIF) glasses, as a subset of metal-organic framework (MOF) glasses, are a newly emerged family of melt-quenched glasses. Recently, ZIF glasses have attracted attention from materials scientists owing to their fascinating properties, such as ultrahigh glass-forming ability, high structural porosity, processability and lack of grain boundaries, and multi-functionality (e.g., gas separation and energy storage). Zn-based ZIF glasses are the most promising MOF glass candidates for large-scale applications. However,

their photonic functionality remains largely unexplored. In this study, we report the discovery of broadband white light emission in ZIF-62, achieved through a vitrification-pressurization-annealing strategy. In this strategy, visible (blue) light emission emerged after the vitrification of ZIF-62, which is subsequently enhanced and broadened upon pressurization of the ZIF-62 glass. Additionally, a sharp red shift (37 nm) of the emission peak occurred in pressurized ZIF-62 glass as the annealing temperature exceeded a critical annealing temperature (1.07T_g). This implies that the photoluminescence behavior of ZIF-62 can be precisely tailored by this strategy. The photoluminescence quantum yield of ZIF-62 glass reached 12.2% after annealing at 1.13T_g for 30 min. The origin of the observed phenomena was revealed by conducting structure analyses. Based on the annealed ZIF-62 glass with the best performance, we fabricated a white light-emitting diode (LED) with a luminous efficacy of 4.2 lm/W and high operational stability, retaining 74.1% after 180 min of operation. This study demonstrated the feasibility of utilizing ZIF-62 glass in LED applications and a significant advancement in the development of one-component white LEDs.

Thermally and Optically Induced Johari Goldstein (JG) Relaxation in As₂Se₃

Muhammad Umair, Department of Physics and Astronomy "Galileo Galilei", Univeristy of Padova, Italy

In numerous fragile glass-formers, as organic and metallic ones, the signature of the JG relaxation is clearly visible in several spectroscopies. This is not the case for many strong glass formers, such as chalcogenides (CGs) and oxides. In an enthalpy relaxation experiment, we found calorimetric evidence of the JG relaxation in a fast quenched (3200 K/s) As₂Se₃ glass, which is not there if a slowly cooled (1 K/s) glass is inspected instead. KWW-fitting was used to obtain values for the relaxation time and stretching coefficient for the JG process [1]. Furthermore, recently, due to their strong photosensitivity and cost-effective optical designs, CGs have attracted significant attention. Photo-relaxation effects impact significantly the stability of these materials, which is crucial for their applications in devices. Therefore, I performed irradiation experiments on the As₂Se₃ CG demonstrating that light has a strong effect on the glassy matrix and can induce either rejuvenation or relaxation in the glass. In particular, I observed strong enthalpy changes for differently quenched glasses studied with a single optical power density (Pd), revealing that a unique iso-enthalpic state is reached after a sufficiently long irradiation time. Interestingly, this unique state is characterized by a fictive temperature (T_f) of ~1.2T_g: for lower T_f, glasses only exhibit rejuvenation upon irradiation; for higher T_f, conversely, only show annealing. This complements nicely the results of a recent report for an X-ray irradiated chalcogenide glass [2], which showed only rejuvenation.

References: [1] Muhammad Umair et al. "Calorimetric signature of Johari–Goldstein relaxation in fast-quenched As₂Se₃". *Thermochimica Acta* (2025).

[2] Jacopo Baglioni et al. "Uniqueness of glasses prepared via x-ray induced yielding". *Reports on Progress in Physics* 87.12 (2024).

Composition-Dependent Viscoelastic Deformation Behaviors of Ge-Se-Te Glass for Use as Molded Lenses

Iljung Yoon, Korea aerospace university

For the advanced driver assistance system (ADAS) installed in a motor vehicle to be better functioning, its cognitive performance during nighttime and/or under adverse weather conditions needs to be further enhanced by way of adopting thermal cameras. The recently mandated safety regulations aimed to improve detection ability of the vulnerable road users have also spurred the integration of thermal cameras. Contrary to the representative single-crystalline Ge ingot which suffers from the cost issues related to the crystal growth process as well as the lens machining process, chalcogenide glasses are not only molding-process

compatible in production of infrared imaging lenses but also compositionally flexible in control of macroscopic optical/thermal properties. As such these attributes enable cost-effective mass production of aspherical refractive lenses. Here, it is noteworthy that the commercially available chalcogenide glasses for use as long-infrared imaging lenses are basically selenide glasses, so that their optical properties such as refractive index and dispersion are limited in designing the lens assembly. Te-based chalcogenide glasses can exploit the merits stemming from the high polarizability of Te atoms. Ternary Ge-Se-Te system is particularly attractive in terms of its glass forming ability as well as high refractive index and low refractive index dispersion. Viscoelasticity inherent in glass materials is a key enabler that realizes the precision glass molding (PGM) process in production of imaging components. In this regard, viscoelastic deformation behaviors in addition to relaxation characteristics of Ge-Se-Te glass need to be analyzed to better assess its PGM compatibility. In this study, composition dependence of viscoelastic deformation of Ge-Se-Te glasses has been addressed in an effort to elucidate influences of Te content on the viscoelastic deformation behaviors during PGM process.

Symposium 4: New non-oxide glasses, hybrid glasses and phase-change materials

Chalcogenide Glasses for Advanced Optoelectronic Applications

Changgui Lin, Ningbo University

Among various IR optical materials, chalcogenide glass is the only amorphous material that is transparent from mid-wave IR to long-wave IR, occupying the optical applications of IR thermal imaging, IR photonic chip, and IR sensing that other optical glasses cannot enter into. Besides the excellent optical properties including wide transmission range, large linear/nonlinear refractive index, and low thermal coefficient of refractive index, chalcogenide glass also possesses intriguing acoustic-optic, thermoelectric and ionic conduction properties. The R&D of novel chalcogenide glasses and their applications has become one of the research hotspots both in IR optics and optoelectronics. Here we would like to present a brief report concerning the recent advances of novel chalcogenide glasses and their advanced applications in our research group in Ningbo University.

Advanced chalcogenide glasses and their optoelectronic sensing applications

Shiliang Kang, Ningbo University

Chalcogenide glasses are receiving increasing attention in infrared sensing because of their wide transmission range, low transmission loss, and excellent shaping ability. Besides the superior optical properties, chalcogenide glass also possesses good thermoelectric properties, including high Seebeck coefficient and low thermal conductivity, which is promising for temperature sensing application. Here, I would like to present a brief report concerning the recent advances of novel chalcogenide glasses and their applications in multifunctional sensing.

IR transparent and flexible chalcogenide organic glass

Chengwei Gao, Ningbo University

IR transparent glasses garnered considering attention due to their wide applications in military and civilian fields. However, current inorganic chalcogenide glasses are limited by high density and brittleness, restricting their utilization in emerging flexible and miniaturized infrared optical systems. In contrast, chalcogenide organic glasses (COG), synthesized via inverse vulcanization by copolymerizing elemental sulfur with organic monomers, provide a

compelling alternative. These COG exhibit high infrared transparency, high refractive index ($n \sim 2$), excellent mechanical flexibility, processability, and low cost (utilizing sulfur, a by-product of the petroleum industry). Despite these challenges, the current challenge lies in balancing high sulfur content (>50 wt%), which is necessary for IR transmittance, against thermal stability and mechanical properties. Therefore, this work achieves effective regulation of the optical performance, thermal stability, and mechanical properties of COG via organic monomer structure design (e.g., thiols with different coordination numbers) and the development of novel preparation strategies. Via introducing two monomers with similar structure but different denticity, which are bidentate and tridentate monomer, a COG with remarkable optical transparency in the infrared region (longwave cut-off edge up to $6 \mu\text{m}$) and exceptional flexibility (Young's module down to 0.05 GPa) could be obtained. This flexible and infrared transparent COG is successfully used for focus variable liquid-filled lens and flexible microlens array, which confirming the potential of this COG for applications in a variety of flexible optoelectronic devices. This work provides new material options for applications such as flexible integrated infrared photonics and compact infrared imaging.

Development and Imaging Applications of Infrared Chalcogenide Glasses

Linling Tan, Ningbo University

Infrared thermal imaging technology is increasingly applied across dual-use platforms, including military and security, astronomical observation, medical diagnostics, and industrial inspection. With the rapid advancement of infrared detectors, imaging systems are evolving toward compact, intelligent, and high-performance designs. However, traditional infrared materials like germanium and ZnSe suffer from limited variety and insufficient performance diversity, failing to meet the demands of advanced infrared imaging. To address these challenges, this research clarifies the relationships among composition, structure, and infrared optical, thermal, and mechanical properties of chalcogenide glasses. A multi-dimensional evaluation mechanism is established to synergistically optimize material performance, overcoming bottlenecks in composition design, property enhancement, and fabrication. Innovative methods such as melt casting and 3D printing are developed to produce gradient refractive index and flexible deformable chalcogenide glasses. This work aims to build an independent and controllable innovation system for infrared chalcogenide glass materials, thereby promoting the development of compact, intelligent, and high-performance infrared imaging systems.

Luminescence modulation in Tb/Yb codoped oxyfluoride glass and their glass-ceramic counterparts

Nguyen Mai Phuong Truong, Centre for Functional and Surface Functionalized Glass (FUNGLASS)

Tb³⁺/Yb³⁺ codoped Li-containing oxyfluoride glasses (OxGs) with the composition $47\text{SiO}_2-19\text{Al}_2\text{O}_3-17\text{Li}_2\text{O}-9\text{LiF}-(8-x-y)\text{YF}_3-x\text{TbF}_3-y\text{YbF}_3$ ($x = 0.5, 1, 1.5, 2$; $y = 1, 1.5, 3, 4.5, 5, 6, 7$) were synthesised via the melt-quenching method. Li and F contents were fixed, while Y was substituted by Tb/Yb to investigate concentration-dependent energy transfer. Their glass-ceramic counterparts (OxGCs) were prepared by hot-pressing (HP) glass powder, producing densified samples containing both glassy and crystallised phases under controlled conditions. Differential thermal analysis reveals glass transition temperatures (T_g) of $510-530^\circ\text{C}$ and a thermal stability range of $\Delta T \approx 100^\circ\text{C}$. The Raman spectra exhibit a strong band centred at $\sim 490 \text{ cm}^{-1}$, corresponding to T-O-T (T=Si, Al) bending vibrations. The 27Al-NMR reveals the stabilisation of tetrahedrally coordinated, corner-sharing $[\text{AlO}_4]$ units over octahedrally coordinated ones. The 19F-NMR confirms the presence of Li-F (~ 200 ppm) and Y/Al-F (~ 110 to -130 ppm) environments, indicating a homogenous distribution of F^- in the undoped

glass system. Photoluminescence (PL) spectroscopy under 351 nm excitation demonstrates that higher Tb^{3+} concentration enhances PL intensity, particularly the dominant green emission at 545 nm (Tb^{3+} : 5D4→7F5). The higher Yb^{3+} content strengthens upconversion (UC) emission intensity under near-infrared excitation (980 nm) through cooperative energy transfer processes. The relatively long green-emission lifetimes of Tb^{3+} (~3 ms) in a glass matrix highlight the suitability of these materials for applications such as X-ray scintillation screens, LED phosphors, data encryption... Preliminary HP experiments on powdered glass indicate pressure-assisted crystallisation at ~500°C, leading to the formation of ~15% tetragonal LiREF₄ and 85% hexagonal LiAlSiO₄ nanocrystals embedded in the glass matrix, as confirmed by X-ray diffraction. Although optical transparency decreases (T%OxGs ~80%) to ~20% after sintering, primarily due to carbon contamination and scattering losses, the incorporation of low-phonon-energy LiREF₄ nanocrystals ($h\nu_{ph} \approx 446 \text{ cm}^{-1}$) is crucial for UC-PL and for extending the Tb^{3+} green-emission lifetime. This work has been supported by the VEGA 1/0300/26, VEGA 2/0077/24, and the project PID2024-157258NB-C21 funded by MICIU/AEI/10.13039/501100011033/FEDER, UE.

Tough transparent glass ceramics for multi-mode programmable dynamic tunable persistent luminescence via phase engineering

Yixi Wu, Zhejiang University

Realizing multi-mode programmable dynamic tunable persistent luminescence within a single solid is promising for multi-dimensional information storage and encryption applications. However, coupling luminescent centers with differentiated defect states remains a challenge. Here we report transparent glass ceramics that exhibit photo/thermally dynamic tunable afterglow. A lithium-ion doping-assisted phase separation principle is developed to control the precipitation of defective non-stoichiometric nanocrystals (Zn_{1.7}SiO₄: Li) in glass matrix, constructing a biphasic microenvironment with differentiated defect states. By adjusting the excitation wavelengths (e.g., 254 nm or 365 nm) and charging temperatures (e.g., 298 K or 498 K), the programmability of the trap states in dual-phase leads to a relative intensity change of the dual emissions, making spatiotemporal tunable PersL of wide chromaticity from orange to green. The developed transparent composites exhibit excellent hardness of up to 10 gigapascal and high thermal stability, which is applicable for harsh conditions. This work pioneers a strategy for modulating dynamic afterglow in a single solid and inspires more potential applications in multi-dimensional information storage and encryption.

Multiresponsive glasses

Lothar Wondraczek, University of Jena

Physical properties arise from a material's response to external stimuli. Under certain conditions, for example, when response reactions are highly non-linear, this can lead to extreme situations, often perceived as switching or material adaption. Irreversible reactions can be used for material conditioning and training, and reversible reactions lead to memory effects. Materials exhibiting such phenomena are often termed smart or intelligent, and are mostly found among compounds with weak, supramolecular bonding states. Multiresponsivity, that is, stimulus-response involving two or more inharmonic or opposite response reactions, enables logical operations. In this presentation, some examples and conditions will be discussed as to how the more stable inorganic and hybrid glasses can still be used as programmable materials with the ability to adapt to certain environmental conditions.

Towards Additive Manufacturing of Far-Infrared Optics

Pierre Lucas, University of Arizona

Telluride glasses are the only class of amorphous solid that retain high transmissivity in the far infrared region past 20 μm . Thus they are key to the design of technologically relevant optical systems such as night vision imaging or communication through the second atmospheric window. Conventional infrared glass optics are produced by melt-quenching followed by molding, thus limiting the geometrical complexity of optical elements and the range of accessible compositions. Here we present a solution-based approach for the production of amorphous tellurides that not only yields glass stoichiometries that are not accessible through conventional melt-quenching methods, but is also compatible with the fabrication of glass optics through additive manufacturing. Various Ge and As based telluride glasses with compositions laying outside of the normal glass-formation domains are produced following a low temperature route that does not involve melting. The process is based on a combination of mechano-synthesis and dissolution in amine and thiol solvents followed by spin coating. Multilayer deposition of telluride glass with seamless interface is demonstrated and the resulting glass films are shown to have excellent optical transparency in the far infrared.

Pressure–Temperature Driven Structural Evolution Across Polyamorphism in Phase-Change Materials

Shuai Wei, Aarhus University

Phase-change materials (PCMs) such as Ge–Sb–Te alloys can rapidly and reversibly switch between amorphous and crystalline states, enabling emerging electronic and photonic technologies. Beyond this well known functionality, PCMs also exhibit polyamorphism in glassy and liquid states, including a high density-to-low density transformation and an associated metal-to-semiconductor transition accompanied by a pronounced dynamical crossover in viscosity consistent with a fragile-to-strong transition. Here we combine high pressure synchrotron X-ray scattering with femtosecond X-ray free electron laser (XFEL) diffraction to map amorphous structure across a broad pressure, temperature, and compositional space. We track the structural evolution through the polyamorphic transition and identify clear signatures in short range order, including the Peierls-like distortions in local octahedral motifs, together with evolution in medium range order. We further show how these structural fingerprints evolve systematically with pressure, temperature, and composition, and interpret the results within a two state model framework, drawing a close analogy to polyamorphism in glassy water.

Biomolecular Noncovalent Glasses: Fabrication Fundamental, Multifunctional Properties, and Emerging Applications

Yang Li, Ningbo University

Supramolecular glasses, as an emerging class of noncovalently cross-linked amorphous materials, have attracted extensive attention in materials science due to their inherent modular structures and dynamic adaptability. Biomolecular noncovalent glasses (BNGs), constituted from amino acids, peptides, and derivatives through dynamic noncovalent interactions, constitute an emerging class of supramolecular glasses. In this review, we begin by introducing the fundamental amorphous structure and synthesis methods of BNGs. We then summarize the latest advances in understanding their glass formation mechanisms, thermodynamic property, mechanics property, optical property, and biology properties. We also explore their potential applications in photonic and optical engineering, biomedical engineering, and environmental engineering. Finally, we analyze the significant challenges faced in the practical application of BNGs and investigate the potential of developing BNGs through the integration of machine learning and multifunctional hybrid systems. This review

aims to draw the scientific community's attention to BNGs' research, summarize the latest advances in the field, and promote further development in this area.

Symposium 3: Glasses for health and green energy technology

Silicates: Paving the Way for Biodegradable Glasses in Tissue Regeneration

Leena Hupa, Åbo Akademi

Most commercially available bioactive glasses used in implantable medical devices are classified as phosphosilicate glasses. These glasses are generally biodegradable and consist of oxides of silicon, phosphorus, calcium, and sodium, i.e., elements that are common in the human body. A key feature of these glasses is their ability to support the formation of hydroxyapatite surface layers in vivo. This property facilitates direct chemical bonding between the implanted glass and biological apatite present in living bone. Advancements in biomedicine have revealed that the composition of glass and its ability to release its constituent elements into the surrounding solution are crucial for tissue regeneration. This discovery, combined with an improved understanding of how different elements interact with biological processes, has enabled the incorporation of additional elements into bioactive glasses. This presentation reviews key considerations for adjusting silicate glass compositions to facilitate the production of desired hot-worked forms and to control biodegradation. Additionally, the role of phosphorus in silicate glasses with respect to bioactivity will be revisited. Comparisons with systems other than silicate glass will also be discussed. The aim is to highlight the key requirements to be considered when designing innovative glasses for implantable devices.

Bioactive Glass for Improved Oral Care

Qiang Fu, Corning Incorporated

Bioactive glass, invented in 1960s, was initially targeted for soft tissue or non-loaded hard tissue regeneration. More recently, research has been conducted to explore their applications in vascularization, wound healing and beyond. To meet the requirements for these emerging applications, glasses in the form of particulates, microspheres, fibers, and porous scaffolds have been developed. Meanwhile, exploration of new glasses with a step change in bioactivity and performance is critical to enable new applications. In this talk, our recent progress on glasses for oral care will be covered; and their performance, at both component and product levels, will be discussed.

Bouncy Bioglass – a new hybrid material for tissue regeneration

Francesca Tallia, Imperial College London

In this talk I will present a new bioglass-based material for the treatment of osteochondral defects. These involve damage to both articular cartilage and subchondral bone. There is unmet clinical need for devices to regenerate articular cartilage because adult cartilage cannot heal itself. 66% of patients with knee pain have cartilage defects and 300k patients undergo surgery annually for such defects in the USA alone [1]. We patented a silica/polytetrahydrofuran/polycaprolactone sol-gel hybrid, named "Bouncy Bioglass". This is an interpenetrating co-network of organic and inorganic components that can be 3D printed into porous scaffolds with controlled porosity and tuneable mechanical properties, with ability to stimulate articular cartilage regeneration [2, 3]. Adding calcium cations to the inorganic component made it tough and bioactive, with the ability to stimulate apatite deposition in vitro [4, 5]. We designed an osteochondral implant achieved by 3D printing a chondral device, with a bulk articular surface bonded to a 3D printed scaffold both made of Bouncy Bioglass, joined to a bone scaffold, made of the Ca-containing Bouncy Bioglass. The main challenges are:

achieving a successful bond of the three components; having the lowest possible friction coefficient against living cartilage; guiding stem cells to produce high quality articular cartilage or bone in the corresponding part of the device. The talk will explore the research from the invention of the material to the additive manufacturing of a device, and the first steps in the translation from lab to industry. This includes a complete mechanical and morphological characterisation of the cartilage and the bone components and the biological response in vitro and in vivo in sheep.

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Symposium 1: Fundamentals of glasses: formation, structure and physical properties

The material-time concept in physical aging

Jepe Dyre, "Glass and Time", Dept. of Science & Environment, Roskilde University

This talk presents experimental and simulation data on physical aging, which illustrate and validate the old concept of a "material time" controlling aging. The beautiful idea behind this of Narayanaswamy (1971) [1] is that the highly nonlinear aging phenomenon can be described in terms of standard linear-response theory if time is replaced by material time. In the case of a temperature down jump from a state of equilibrium, the clock rate gradually decreases to eventually reach the equilibrium relaxation rate characterizing the final temperature. We present data confirming this approach to physical aging and relate the material-time concept to the ground-breaking triangular relation of Kurchan and Cugliandolo (1994) [2]. The experimental data presented include the first direct test of Narayanaswamy's approach (from accurate dielectric measurements) [3], as well as light-scattering data establishing "material-time reversibility" [4]. Supplementing this, simulation data will be presented that illuminate a "distance-as-time" interpretation of the material time [5]. The latter data show that aging is controlled by how fast the slowest particles move. This very recently led to the concept of "double percolation" controlling the alpha and beta relaxations of equilibrium (metastable) glass-forming liquids [6], which is briefly reviewed if time allows.

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Geological timescales' aging effects of lunar glasses

Ziqiang Chen, Dongguan Institute of Materials Science and Technology, Chinese Academy of Sciences

Physical aging is a long-lasting research hot spot in the glass community, yet its long-term effects remain unclear because of the limited experimental time. In this study, we discover the extraordinary aging effects in five typical lunar glassy particles with diameters ranging from

about 20 to 53 micrometers selected from Chang'e-5 lunar regolith. It is found that geological time scales' aging can lead to unusually huge modulus enhancements larger than 73.5% while much weaker effects on hardness (i.e., varies decoupling evolutions of Young's modulus and hardness during aging) in these lunar glassy samples. Such extraordinary aging effects are primarily attributed to the natural selected complex glassy compositions and structures, consistent with high entropy and minor element doping criteria, prevailing under the special lunar conditions and the extensive aging time for the lunar glasses. This study offers valuable insights for developing high-performance and stable glassy materials for radiation protection and advanced space explorations.

Atomic-scale simulations of the mechanics of real-world glasses at experimentally accessible time-scales

Ankit Singh, University of Milan

While classical elasticity theory describes the mechanical deformation of solids without any reference whatsoever to the atomic constituents of matter, modern lattice dynamics provides quantitative ways to compute elastic constants in terms of atomic-scale configurations and interactions. Within this framework, the fundamental problem is reduced to evaluating forces and configurations in MD simulations. Nonetheless, for real solids (incl. crystals with defects and grain boundaries, non-centrosymmetric crystals, heated crystals, glasses), the elasticity is dominated by relaxational atomic motions that are not included in standard (Born-Huang) lattice dynamics [1-4]. These atomic motions are referred to, in the current literature, as “nonaffine motions”: they are associated with incompatible deformations, and are ubiquitous in real-life materials. In general, since they stem from the relaxation of local interatomic forces due to the lack of inversion symmetry, the nonaffine motions are linked to a significant decrease (softening) of the elastic constants, in particular the shear modulus. For example, nonaffine motions can quantitatively explain the mechanics of diverse systems such as the jamming transition and marginal elasticity of granular packings [2] as well as the experimentally observed elastic constants of α -quartz [3]. Nonaffine motions can also explain the frequency-dependent viscoelasticity of disordered materials such as polymer glass [4]. This is because, on long time scales, the relaxational nonaffine motions dominate the mechanical response (the zero-frequency plateau modulus), whereas, at high external oscillation frequencies, they become gradually less significant compared to the affine or Born modulus. A recent atomistic implementation of this principle, called NALD (Nonaffine Lattice Dynamics), provides a new way to solve the time-scale bridging problem of glass mechanics [5,6], whereby traditional atomistic MD simulations are strongly limited by the simulation time-step, and its predictions are confined to deformation frequencies/time-scales that are too high to be accessible experimentally. Because NALD leverages the direct diagonalization of the Hessian matrix of the solid, it is perfectly feasible for the atomic-level description of the mechanical properties of nanostructured materials, in combination with the state of the art in interatomic forces and interactions. We will show how NALD can provide atomistic computational predictions of elastic moduli of chemically-complex glasses in parameter-free agreement with experimental data of mechanical testing (e.g. Dynamic Mechanical Analysis) [5-7] as well as with Brillouin spectroscopy measurements.

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Shaping Glasses with X-rays

Giulio Monaco, Department of Physics and Astronomy, University of Padova, Italy

Illuminating an insulating or semiconducting glass using X-rays changes the properties of the glass, even when low dose and dose-rates are used. The reason behind this is the complexity of the energy landscape of glasses, characterized by a huge number of different minima: during x-ray illumination the glass becomes an active system, powered by the absorbed energy, and explores this landscape. An x-ray illuminated glass becomes then the playground to study, under controlled conditions, phenomena which also appear in other contexts. On the basis of x-ray scattering and x-ray photon correlation spectroscopy combined with nanocalorimetry experiments, I will discuss how x-ray irradiation can be used to prepare rejuvenated, high-enthalpy glasses [1,2]. In particular, while enthalpy increases with irradiation in a first stage, a sufficiently long irradiation results in a stationary state, independent of the initial state of the glass. The transition to this stationary state corresponds to the yielding transition [3].

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Elucidating the features of the Boson peak to expand upon the understanding of amorphous phase-change materials

Jens Moesgaard, Aarhus University, Department of Chemistry

Phase Change Materials (PCM) are promising candidates for applications in switchable non-volatile memory, photonic, and neuromorphic computing devices due to their fast phase switching between crystalline and amorphous states, accompanied by a high electrical and optical contrast. Yet, at elevated temperatures, these phase changes are so fast that they obfuscate characterizations of the amorphous states using conventional thermal analysis, necessitating newer avenues of analysis. A recent study of ours demonstrated how modeling the low-temperature heat capacity phenomena known as the “Boson peak” enables such an avenue for thermodynamic analysis of amorphous materials, through a comprehensive analysis of oxide-, chalcogenide-, and metallic glasses. The Boson peak is a universal yet elusive property of all amorphous materials; as such, ascertaining the underlying features of the Boson peak and how they relate to other amorphous properties has been of interest for over 50 years. The Boson peaks were modeled through a 4-parameter fitting equation, which attributes the Boson peak to hybridized vibrations from locally favoured structures called “dynamic defects”. These fitting parameters were shown to correlate with the glass transition temperature and the kinetic fragility index depending on whether the glass was predominantly covalent or metallic. Presently, we have incorporated a broad range of PCMs, including the archetypical PCMs: GeTe, Ge₂Sb₂Te₅, and Ge₁Sb₂Te₄ from the Yamada line, as well as Ag₄In₃Sb₆₇Te₂₆ (AIST) and Ge₁₅Sb₈₅ into the analysis. Additionally, chalcogenide GeSeTe glasses were also included. This comprehensive analysis of Boson peaks, glass transition behaviors, and fragilities gave additional evidence for their interrelations, consistent with earlier Boson peak studies. In addition, investigations into cross-correlations between fitting parameters revealed a more detailed interpretation of the Boson peak’s origin.

In-Situ XRD Tracking of Structural Changes in Metallic Glasses During Thermal Scans

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Understanding atomic-scale structural changes under varying thermodynamic conditions is essential for studying material properties and the mechanisms governing them, particularly in

glasses where thermal history plays a critical role. To address this, we developed a novel experimental setup combining synchrotron X-ray total scattering with fast differential scanning calorimetry (FDSC) [1], enabling in-situ characterisation of nanoscale structural transformations during and after rapid thermal scans. The low-background sample environment ensures high-quality X-ray diffraction data, allowing for detailed analysis of different amorphous states. Using this approach, we tracked the temperature-dependent evolution of a Pd-based metallic glass (Pd_{42.5}Cu₃₀Ni_{7.5}P₂₀) during controlled FDSC protocols. Clear and reproducible atomic-scale changes were observed on millisecond timescales and across cooling rates from 1 K/s to 10⁴ K/s, enabling direct correlation of structural response with both temperature and quenching rate. The measurements also allowed quantification of X-ray beam-induced heating, confirming that the observed changes reflect intrinsic material behaviour. Aging experiments at temperatures near the glass transition further revealed how thermal history and the initial enthalpic state influence structural relaxation. Overall, these results provide new insights into the interplay between atomic structure and thermodynamics in metallic glasses, and demonstrate the potential of this approach for systematic studies of other disordered systems.

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Bond Angles and The Structure of Vitreous Beryllium Fluoride

Alex Hannon, ISIS Facility

Vitreous BeF₂ has a structure formed of corner-sharing BeF₄ tetrahedra, which appears to be similar to that of vitreous SiO₂. The strength of Be-F bonds is much less than that of the Si-O bond, and thus BeF₂ may be considered a weakened analogue of SiO₂. BeF₂, however, is much less studied than SiO₂ due mainly to its high toxicity. A report is given of a neutron diffraction study of the structure of vitreous BeF₂, with particular emphasis on the bond angle distribution (BAD), both in BeF₂ and in other similar systems. The first report of an attempt to determine the BAD in a glass, was an X-ray diffraction study by Mozzi and Warren. Diffraction methods should be playing an important role in the study of the BAD, but almost all subsequent reports have been based on NMR results, possibly due to the difficulty of the calculations for modelling the effect of the BAD on diffraction results. An algorithm has been developed for these calculations, and the first report of its use is given, in which it is applied to neutron diffraction results for BeF₂.

Design and analysis of local structures of halide perovskite nanocrystals in glasses

Ruilin Zheng, Nanjing University of Posts and Telecommunications/Shanghai Institute of Optics and Fine Mechanics (CAS)

Metal halide perovskite CsPbX₃ (X = Cl, Br, I) nanocrystals (NCs) have attracted great attention due to their excellent properties, including high photoluminescence quantum yields (up to 90%), extremely narrow emission width (FWHM <20 nm), and tunable emissions extending the entire visible spectral region. However, the poor stability of CsPbX₃ NCs is still the major matter which hinders their practical applications. In-situ growth of CsPbX₃ NCs in glass matrices improves their stability and opens them up to more potential applications in three-dimensional optical storage devices. Although trial-and-error experiments have improved the performance of the CsPbX₃ NCs in glass matrices in the past few years, it is still difficult to design and control the properties of the CsPbX₃ NCs in amorphous matrices. Therefore, it is very important to design and analysis of local structures of halide perovskite NCs in glass matrices. In this work, we clarified the in-situ growth mechanism of halide perovskite NCs in amorphous matrices and proposed an adjustable self-straining strategy to

control their temperature and pressure co-induced phase transitions. We proved that there are five phases (monoclinic, orthorhombic, tetragonal, cubic, and amorphous) for CsPbBr₃ NCs in glasses, and there is a dynamical process combining compositional segregation (mixing) and structural disorder (order) for mixed-halide CsPbX₃. Most importantly, the encapsulation of CsPbBr₃ NCs in a glass matrix excludes the effect of external environments allowing us to elucidate the widely existing “self-straining effect” for heterostructured NCs and phase segregation for mixed-halide perovskite. This work provides a better fundamental understanding of the phase transitions of halide perovskite NCs and paves the way toward the development of an in situ method to predict the multi-physical variables co-induced structural evolution of halide perovskite NCs in optoelectronic devices.

Additive Manufacturing of ZBLAN Fluoride Glass via Fused Filament Fabrication

Johann Troles, University of Rennes

Fluoride glasses such as ZBLAN are distinguished by their low dispersion, high transmittance, and wide transparency window in the mid-infrared (mid-IR) region, making them promising candidates for optical fiber technologies, infrared spectroscopy, and mid-IR laser systems. Despite these advantageous optical properties, the fabrication of fluoride-based components remains challenging due to their sensitivity to crystallization and stringent processing requirements. In this work, we investigate the feasibility of fabricating ZBLAN glass via fused filament fabrication (FFF) as a route toward additive manufacturing of infrared optical materials. High-purity ZBLAN rods were synthesized and characterized to establish suitable thermal processing windows. By tuning extrusion temperatures and printing parameters, we achieved the successful layer-by-layer deposition of fluoride glass using an FFF platform. The amorphous nature of the printed material was confirmed, and transmission measurements revealed values exceeding 50%, demonstrating the preservation of optical transmission after printing. These results highlight the potential of additive manufacturing for fluoride glasses and open avenues for the development of customized mid-IR optical components, fiber preforms, and microstructured glass architectures.

Multiscale Structural Disorder in Glasses: Beyond Local Coordination Effects on Rare-Earth Ion Luminescence

Qi Zhang, Nanjing University of Posts and Telecommunications

Disentangling how structural disorder at different length scales governs rare-earth luminescence remains a fundamental challenge in optical materials science. Although local coordination environments are widely regarded as the primary determinants of rare-earth emission, growing evidence indicates that structural organization beyond the first coordination shell can also play a critical yet insufficiently understood role. In crystalline materials, however, the intrinsic requirement of long-range periodicity severely constrains the introduction and independent control of disorder, limiting systematic investigations across multiple structural length scales. Glasses provide a unique structural platform to overcome this limitation, as they inherently combine long-range disorder with tunable short- and medium-range organization. In this work, Ce³⁺-doped borosilicate glasses are employed as a model system to investigate the distinct roles of short-range and medium-range structural disorder in regulating rare-earth luminescence. By systematically varying the B/Si ratio, the glass network structure is modulated in a controlled manner, enabling selective tuning of different structural regimes. Advanced structural characterization, including synchrotron-based pair distribution function analysis, reveals contrasting structural responses at different length scales, highlighting the nontrivial evolution of medium-range order within the disordered glass network. Complementary optical and temperature-dependent spectroscopic measurements demonstrate that the observed luminescent behavior cannot be fully accounted for by local coordination effects alone. Instead, it reflects a coupled response to structural organization

extending over multiple length scales. In particular, variations in medium-range structural flexibility are found to correlate with distinct thermal response characteristics, suggesting an important role of non-local structural effects in governing non-radiative relaxation processes. Together, this study proposes a hierarchical perspective on rare-earth luminescence regulation, in which short-range and medium-range structural disorder play fundamentally different yet cooperative roles. These findings provide new insight into disorder-sensitive luminescence mechanisms in glasses and offer general guidance for the rational design of luminescent materials through controlled structural complexity.

Bond counting strategies in an oxygen centric perspective on the structure of oxide glasses

Philip Stephen Salmon, University of Bath

Bond counting strategies provide a simple but robust method for examining the connectivity of the network forming motifs in oxide glasses. This utility is demonstrated for several case examples in which diffraction is combined with solid-state NMR and other methods to probe the glass structure. The approach is used to show that four-coordinated Zn²⁺ and Mg²⁺ ions act as network modifiers in alkali bearing metasilicate glasses. Analytical models are then derived for the structure of mono- or di-valent cation containing aluminosilicate glasses in which the fraction of six-coordinated Al³⁺ ions is negligibly small and the other aluminium species are regarded as network formers. The results lead to an assessment of the network modifying versus charge compensating roles of the Zn²⁺ and Mg²⁺ ions. Next, the effect of high-pressure on the network connectivity of aluminosilicates is investigated, leading to a quantification of the fraction of triply bonded oxygen atoms (or oxygen triclusters) in fully polymerised structures. A network forming role is then found for six-coordinated Nb⁵⁺ ions in the binary Nb₂O₅-NaPO₃ system. Finally, it is noted that the oxygen packing fraction acts as a marker for structural change in network-forming oxides under high-pressure conditions. The findings illustrate the power of the bond-counting methodology in elucidating the structure of amorphous oxides and show the rich diversity in framework structures that originates on progressing from a Zachariasen viewpoint of oxide networks.

Predicting Contents of Non-Bridging Oxygens and Oxygen Triclusters in Aluminosilicate Glasses From ²⁷Al NMR Data

Mattias Edén, Stockholm University

We demonstrate that the entire set of bridging oxygen (BO), non-bridging O (NBO), and O tricluster populations may be deduced for an aluminosilicate (AS) glass by knowledge of its composition and the {AlO₄, AlO₅, AlO₆} populations that are readily extracted from routine ²⁷Al magic-angle-spinning (MAS) nuclear magnetic resonance (NMR) experiments. The procedure typically reproduces previously published NBO fractions derived by ¹⁷O MAS NMR experiments within ±0.02, which is almost within experimental uncertainties. Yet the primary utility of the method is for the vast majority of AS glasses for which expensive ¹⁷O enrichment is not available, and notably so for glass systems where the ¹⁷O MAS NMR spectrum manifest significant overlap between the resonances from the BO and NBO sites, such as AS glasses comprising Li⁺, Na⁺, and Mg²⁺. Oxygen triclusters, which coordinate three network-forming cations, was proposed 60 years ago and has since then been heavily debated because direct and irrefutable experimental proof for their existence is still lacking in AS glasses. Although O triclusters were originally proposed for balancing the negatively charged AlO₄ groups that typically dominate the Al speciation in AS glasses, computational modeling reveals the strongest propensity for their accommodation at the high-coordination AlO₅ and AlO₆ polyhedra. We highlight the close structural relationship between the O triclusters and AlO₅/AlO₆ polyhedra, where evidence is piling up for a network-forming role of the high-coordination Al species.

Lanthanum Stabilized Cubic BaCl₂:Eu²⁺ Nanocrystals in Glass with Enhanced Photoluminescence and Scintillation Performance for High-resolution X-Ray Imaging

Wei Zhang, Zhejiang University

Dopant-activated glass ceramics (GCs) are emerging scintillation candidates for X-ray imaging and detection. Their scintillation performance is mainly determined by the local structure (coordination environment, bonding arrangement, etc.) of dopants, but the structure of nanocrystals (NCs) in glass is relatively hard to manipulate in a controlled manner. Herein, we demonstrate that LaCl₃ incorporation in fluorophosphate-aluminate glass can control the phase transition of BaCl₂ NCs and engineer the chemical environment of Eu²⁺ dopants, inducing tunable peak position and enhanced photoluminescence (PL) quantum efficiency simultaneously. Benefiting from the local atomic arrangement of lanthanum stabilized cubic BaCl₂:Eu²⁺, narrow-band emission located at 420 nm with high internal/external quantum efficiency (87.2%/61.9%) is realized. Owing to the protection of a robust glass matrix, GCs show long-term water resistance (75% PL intensity retention after 150 days of water immersion) and good thermal stability (60% PL intensity retention at 423 K). By tuning the crystallinity, GCs either exhibit 190.5% radioluminescence intensity compared to Bi₄Ge₃O₁₄ or a high spatial resolution of 17.1 lp mm⁻¹. Furthermore, the detection limit is as low as 140 nGy s⁻¹, and the X-ray imaging is demonstrated with target objects. These findings provide new insights into the phase control of NCs in glasses with enhanced scintillation performance for high-resolution X-ray imaging applications.

Abstracts - Wednesday June 17

Plenary session

From Augmented Reality to Laser Fusion: Glass at the Core of Future Technologies

Sebastian Leukel, Development SCHOTT AG

Glass is a key enabler for advanced optical and photonic technologies addressing global trends in augmented reality (AR), high-performance computing, and sustainable energy. Its unique combination of transparency, tunable refractive properties, and processability positions glass at the center of next-generation systems. High-refractive-index glasses are critical for AR optics, where high optical performance must be combined with low density for user comfort. Achieving this requires compositional design strategies that push the limits of glass formation while maintaining highest transmission. In integrated photonics, femtosecond-laser writing enables direct inscription of low-loss waveguides and complex three-dimensional photonic circuits within glass substrates. This approach provides a scalable route for photonic integrated circuits (PICs) used in AI acceleration, quantum computing, and high-speed data transmission. For high-energy applications, rare-earth doped laser glasses serve as gain media in high-power laser systems, delivering the energy densities required for inertial confinement fusion (ICF). Their tailored spectroscopic properties and mechanical robustness are essential for achieving the stringent performance targets of laser-driven fusion. Furthermore, luminescent glasses bearing perovskite quantum dots and other inorganic nanoparticles are at the center of much current attention for applications such as solar light conversion towards improvement of PV cells, photocatalysis, and solid-state lighting. Particle embedded optical fibers have been equally largely pursued for the development of integrated photonic devices and enhanced sensing/biosensing. Combining tunable properties with scalable processing, glass remains a fundamental material for all kinds of emerging optical and photonic technologies.

Ultrafast laser induced order/disorder changes and applications

Jianrong Qiu, Zhejiang University, China

Femtosecond laser is an extreme physical condition which can be realized in normal laboratories. It has been widely used for microscopic modifications to materials due to its ultra-short laser pulse and ultrahigh light intensity. When a transparent material is irradiated by a tightly focused femtosecond laser, the photo-induced reaction occurs only near the focal point of the laser beam inside the material due to the multiphoton processes. In this talk, we will describe our observations of various phenomena related to order/disorder change in transparent materials. The mechanisms and promising applications of these phenomena for optical memory with ultrahigh storage density, micro-spectrometer, micro-LED array are also discussed.

Symposium 3: Glasses for health and green energy technology

Thin-Film Li Glassy Solid Electrolytes as a New Functionality for Glass Enabling High Energy Density Li All Solid State Batteries

Steve W. Martin, Iowa State University of Science & Technology

Fast ion conducting glasses have long been considered as alternatives to flammable liquid electrolytes in Li batteries. However, to date, there has never been before the unique combination of required electrochemical properties in any one such glass for its use as a solid electrolyte with the equally important requirements of viscoelastic behavior and strong resistance to crystallization to form them into thin films suitable for high ion conductivity separators. In this first ever report of thin film fast ion conducting glasses, we will summarize our efforts to produce thin films of Li ion conducting glasses and test in them in symmetric, asymmetric, and full cells.

Engineering a Stable Electrode-Electrolyte Interface via Glass Structural Affinity for High-Performance All-Solid-State Lithium-Ion Batteries

Yanfei Zhang, Qilu University of Technology

All-solid-state lithium-ion batteries (ASSLIBs) are promising candidates for next-generation energy storage due to their high energy density and intrinsic safety. However, their practical application is hindered by insufficient ionic conductivity of solid electrolytes and poor electrolyte-electrode interfacial compatibility. Herein, we address this fundamental challenge by designing a novel “glassy battery” where a vanadium phosphoborate (VPB) glassy electrode is seamlessly integrated with a Sn-doped NASICON-type glass-ceramic electrolyte ($\text{Li}_{0.5}\text{Al}_{0.5}\text{Sn}_{0.4}\text{Ti}_{1.1}(\text{PO}_4)_3$, LAMP-S4-1000-10). This integration is achieved by developing a “structural affinity” between the disordered glassy electrode and partially disordered glass-ceramic electrolyte, which facilitates an intimate, low-impedance interface without compromising ionic conductivity. The optimized LAMP-S4-1000-10 electrolyte exhibits a high ionic conductivity of $1.15 \times 10^{-4} \text{ S cm}^{-1}$ and a low activation energy of 0.23 eV for Li^+ diffusion. Benefiting from this uniquely engineered interface, the resulting Li//LAMP-S4-1000-10//VPB full cell delivers an impressive capacity of 228 mA h g⁻¹ after 500 cycles at 0.1 A g⁻¹, coupled with the superior rate capability and long-term cyclability. This work provides a paradigm-shifting strategy to overcome interfacial challenges in ASSLIBs through synergistic glass-based material design, offering a new perspective for solving interface issues in all-solid-state energy storage systems.

Engineering a Meltable MOF to Tune Liquid Transition and Promote Coenzyme Regeneration

Wengang Huang, The University of Queensland

Modulating the liquid phase of metal–organic frameworks (MOFs) presents new opportunities for functionalizing glassy MOFs, expanding the fundamental science and practical application for this emerging family of materials. Herein, we report the fabrication of a bimetallic glassy MOF via a liquid–liquid transition process. This is achieved by introducing a robust Schiff base–cobalt functional group into Zn-ZIF-62, which attracts negatively charged imidazolate ligands, facilitating low-temperature melting. This ultimately leads to the formation of a bimetallic glassy MOF (Co/Zn-agZIF-62-ipy) upon melt-quenching. The material features an exceptionally high glass-forming capability, uniformly distributed bimetallic ions, and a markedly enhanced visible light photogeneration efficiency of enzymatically active nicotinamide adenine dinucleotide (NADH) when compared with Co-doped ZIF-62 glass. These findings offer novel insights into modulating the liquid phase of an MOF to develop

functional glassy MOF photocatalysts for coenzyme NADH regeneration and other advanced applications.

Structural origins of high MoO₃ solubility in peraluminous borosilicate glasses

Ashutosh Goel, Rutgers, The State University of New Jersey

Molybdenum imposes strict solubility limits in conventional borosilicate nuclear waste glasses due to the tendency of tetrahedral molybdate (MoO₄²⁻) species to phase separate and crystallize as alkali molybdates. Here, we demonstrate an unprecedented 13.96 wt.% (7.51 mol%) MoO₃ solubility in peraluminous sodium aluminoborosilicate glasses—a ~15× increase over their peralkaline counterparts. Using Raman spectroscopy, multi-nuclear and dipolar-correlation MAS NMR, EPR, and STEM-EDS, we reveal that Na-deficient, low-optical-basicity conditions stabilize octahedral MoO₆ units, which polymerize into molybdite-like Mo–O clusters dispersed within the glass matrix. These Mo-rich clusters suppress the formation of depolymerized [MoO₄]²⁻ environments typically responsible for Na₂MoO₄ precipitation and instead promote the formation of Na₂Mo₂O₇ as the saturation phase. Concurrently, Mo incorporation drives the conversion of AlO₄⁻ to higher-coordination AlO₅ species, liberating Na⁺ that is subsequently sequestered into molybdate-rich domains. The combined evolution of Mo coordination, modifier redistribution, and network depolymerization provides a mechanistic basis for the markedly enhanced Mo solubility in peraluminous compositions. These findings establish new structural guidelines for designing aluminoborosilicate waste forms with substantially greater capacity to incorporate Mo-rich nuclear waste streams.

Improving Molybdenum Tolerance in Nuclear Waste Glasses: Compositional Modeling and Reduction Strategy

Ziqiang Jia, Wuhan University of Technology

Borosilicate glass remains the predominant matrix material for nuclear waste immobilization. Nevertheless, it exhibits a limited tolerance to molybdenum (Mo), a major fission product, leading to the formation of deleterious molybdate phases. To address this, two complementary approaches were investigated. First, an empirical model was developed based on a dataset of hundreds of crucible-scale experiments to quantitatively predict MoO₃ solubility as a function of glass composition, thereby supporting the design of glass compositions with enhanced molybdenum tolerance. Second, the mechanism of enhancing MoO₃ solubility under reducing conditions was explored by adding tannic acid as a reducing agent during the vitrification process. The Mo species and their local environment were studied using XAS, EPR and molecular dynamics simulations. The results indicate that Mo⁶⁺ within the glass can be reduced to lower valence states including trivalent, tetravalent, pentavalent, and metallic form. The reducing environment weakened the field strength of Mo–O bonds, facilitating the integration of Mo species into the glass network, which, coupled with their more dispersed distribution within the glass, contribute to the observed enhancement in MoO₃ solubility.

The role of ROCKWOOL stone wool production technologies and products in the green transition

Mette Solvang, ROCKWOOL A/S

Decarbonization, sustainability and the circular economy are key components of the green transition. To support this transition, technological innovation and energy savings are needed. It is particularly critical to improve the energy performance of buildings, as a significant portion of the building stock has poor energy performance today. Recently, the EU launched the Energy Performance of Buildings Directive, which addresses the need for renovation of the existing building stock and sets zero emission buildings as the new standard for new

construction. EU countries must also ensure that new buildings are solar ready, meaning suitable for photovoltaic or solar thermal installations. ROCKWOOL stone wool fibres are produced for insulation purposes and remain hidden behind claddings and interior walls for most of their lifetime. The product plays an important role in supporting the comfort of building users, as it insulates against cold and heat, protects against the spread of fire, and enhances the indoor climate. By insulating buildings, less energy is needed for heating and cooling, thereby reducing CO₂ emissions from the built environment. The driver for the ROCKWOOL innovation of production technologies and products is a sustainability strategy covering decarbonization, energy efficiency and circularity, all supporting the green transition. In this presentation, we will illustrate how ROCKWOOL stone wool production technologies and products support the green transition. We will highlight the goal of electrification of the melting process and the consequent decarbonization of production. Furthermore, we will discuss the circularity of the products with regards to recyclability and durability. Finally, we will present examples of products on the market that support the green transition, with respect to both energy savings and fire protection.

Development of in vitro biosolubility test for assessing stone wool fiber biopersistence

Denis Okhrimenko, ROCKWOOL A/S

In this presentation, the recent contribution of ROCKWOOL A/S to European Insulation Manufacturers Association (EURIMA) project for developing MMVF in vitro biosolubility test using acellular dissolution setups will be discussed. Currently, only animal and epidemiological studies are recognized on the regulatory level (Note Q, EC no. 1272/2008) and used for IARC's decision to include MMVFs with low biopersistence into Group 3 (materials not classified for carcinogenicity to humans). Replacement of these animal tests is an important task for new alternative methodology (NAM) strategy. It requires introducing a robust and standardized acellular in vitro dissolution protocol with clear endpoint(s) to draw a correlation with in vivo studies. In our present research, we are exploring applicability of US pharmacopeia apparatus 4 (USP-4) for stone wool in vitro dissolution protocol development, by investigating stone wool dissolution behavior in variety of synthetic lung fluids under different USP-4 operation modes, closed and open loop, representing batch and continuous flow reactors, respectively. These USP-4 dissolution experiments combined with leachate composition measurements give access to stone wool apparent solubility and dissolution kinetic. They can be potentially used as criteria and endpoints for correlation with in vivo data in the future protocol establishment. The results showed that USP-4 experimental conditions significantly influence the dissolution of stone wool, affecting tests endpoint evaluation. To better understand USP-4 results, we also performed single fiber dissolution tests with direct observation of fiber dissolution via optical microscopy. The results of these studies will aid our understanding of stone wool dissolution mechanism and through that also help to further develop acellular in vitro test method for demonstrating in vivo and in vitro correlation for replacing animal tests in the future.

Improving high-temperature stability of stone wool fibres by optimizing crystallisation

Peter Grouleff Jensen, Aalborg University

Stone wool is widely used as a fire-resistant thermal insulation material, playing a crucial role in reducing energy consumption for heating and cooling buildings - a central aspect of the global green transition. Its excellent fire-safety performance is largely attributable to its high-temperature stability (HTS), a property that distinguishes stone wool from glass wool and organic fibers. HTS arises from the unique physical characteristics of stone wool fibers, including a high glass transition temperature and a strong tendency to crystallize upon heating. This presentation provides a comprehensive overview of the current research on the HTS of stone wool fibers. First, the concept of HTS is defined, followed by a discussion of the

experimental and analytical methods used to investigate and quantify this property. Then, various aspects of the crystallisation of stone wool fibers are discussed. These include the surrounding atmosphere, which governs a complex oxidation mechanism; the fibers' chemical composition; and new findings highlighting the effect of glass homogeneity. By providing an overview of the processes governing the HTS of stone wool fibres, this work highlights key areas for research to develop stone wool insulation with improved fire safety, with the potential to aid in the preservation of both property and lives.

Aluminosilicate glasses, weathering and solving the CO₂ challenge

Susan Stipp , DTU-Physics

Weathering of natural solids and dissolution/precipitation of anthropogenic materials are processes that have important economic and health implications in all levels of society, industry and the environment. Geochemists have studied water-rock interactions for decades, including volcanic and impact glasses, but much remains to be understood about the role of organic compounds on such processes. At best, empirical models describe reaction rates but results are unsatisfying because each new system requires its own empirical constants. Improved understanding about the molecular mechanisms controlling the role of organic compounds would contribute to a breakthrough in ability to predict solid-water reactions, which would have broad implications. One implication, that is a core focus of the work in our research group, is the ability of organic compounds to hasten the breakdown of silicate materials, to release divalent cations for trapping CO₂ as carbonate minerals, stabilising the gas as a solid for geologic time. In nature, some organisms produce compounds that “eat” rocks and others produce compounds that enhance precipitation. Our goal is to learn from nature and use its tricks i) to speed silicate dissolution, which would also speed carbonate mineral formation and ii) to control the concentration of Si and Al, which would prevent formation of clays and zeolites, that steal divalent cations from CO₂ mineralisation. Diatoms, single celled algae that trap Si from water at very low concentrations and make glass coverings, might provide a key for forming silica colloids, thus depleting the system of Si needed.

Surface evolution of alkaline silicate materials under ambient conditions

Alexandra Beltrami, DTU Fysik

Mitigating the dramatic increase in CO₂ in air and water requires scalable and durable carbon capture strategies. Basalt and basaltic glass, common alkaline rocks, weather in the presence of CO₂ and water and, with time, lead to stable carbonate phases such as limestone and chalk through divalent cation mineralisation. Alkaline silicate materials, including demolition waste such as stone wool insulation, provide divalent cations, thus offering a promising material for permanent CO₂ storage. Dissolution and secondary mineral formation occur at the solid–air or solid–solution interface so investigating surface evolution is an essential step toward elucidating the mechanisms controlling cation release and the early stages of carbonate formation. We explored the surface behaviour of various types of glass, including industrial soda–lime–silicate and specially made calcium–aluminium–silicate (CAS) as well as natural obsidian and basaltic glass and observed the change in surface concentration during exposure to controlled humidity and CO₂. With X-ray photoelectron spectroscopy (XPS), a technique that probes the top ~10 nm of solids, we monitored changes in surface composition on freshly fractured surfaces, with time. The effect of X-ray beam exposure does not significantly affect surface calcium concentrations, whereas sodium measurably increases, consistent with the higher mobility of alkali species. Exposure to humidity in air at ambient temperature for a week drives cation redistribution: sodium rich obsidian shows surface sodium enrichment, whereas calcium rich CAS exhibits increased surface calcium concentration. This surface rearrangement, even under mild, ambient conditions, influences surface composition, thus reactivity and carbonate formation potential.

Selective leaching of stone wool at high pH by small organic molecules

Santanu Mondal, DTU Physics

Stone wool plays a role in sustainable construction and green energy technologies. As insulation, stability is important whereas if particles are inhaled, rapid dissolution is desirable. In both cases, the activity of organic compounds has an effect on dissolution rate. Waste stone wool has potential as a cation donor in aqueous systems, for trapping CO₂ as carbonate phases but slow dissolution rates make enhanced weathering of stone wool and natural divalent cation aluminosilicate rocks and glass, impractical. If dissolution rates, which are influenced by pH, temperature and the presence of organic compounds could be enhanced, waste stone wool and natural Al-silicates could be used for trapping CO₂. At high pH, hydroxide ions facilitate the degradation of silicate chains, releasing alkali metals and various hydroxide species. Excessive dissolution in a short time can lead to uncontrolled metal leaching (e.g., Ca and Al) and the formation of a passivating layer, which can inhibit further reaction.¹ Chelating ligands are known to influence calcium aluminosilicate dissolution rates under alkaline conditions² but selective element leaching and precise control of the dissolution process remain relatively unexplored. We are investigating the behaviour of small biogenic molecules and their derivatives in controlling selective element leaching (e.g., Ca, Al, Si, Mg). In particular, we have investigated stone wool-water-organic molecule interactions in batch conditions at pH 10 or higher, to understand the molecular level processes by which organic molecules speed silicate dissolution and selectively leach the component elements.

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Surface crystallization of phosphate glass containing CuO and coloring on a float glass

Shujiang Liu, Qilu University of Technology

Crystallization behavior of a phosphate glass containing CuO is investigated. It is found that, when the phosphate glass was prepared under a reducing atmosphere, in addition to phosphate crystals, metallic Cu also was precipitated at the surface of the phosphate glass during heat-treatment around glass transition temperature, thereby exhibiting a metallic luster. This arises from the disproportionation reaction: $2\text{Cu}^+ \rightarrow \text{Cu}^{2+} + \text{Cu}^0$, which takes place at lower temperature compared to crystallization of phosphate phases. Furthermore, the phosphate glass can be used to color the tin-side of the float glass through heat treatment at 600 °C, during which the phosphate glass softened onto the float glass. This helps prevent oxidation of metallic and cuprous species, whose concentration in turn are increased due to the reducing role of tin at the surface of the float glass, whereby the coalescence of Cu and Cu₂O colloids gives rise to ruby coloration.

Symposium 5: Simulations and predictive modelling of glasses

Chiral crystallization of amorphous tellurium

Stephen Elliott, University of Oxford

Tellurium (Te) is one of the very few inorganic materials having a chiral (in this case helical) crystal structure. However, the mechanism(s) by which chirality occurs on crystallization is unclear. In this talk, I will describe the results of computer simulations of the crystallization of glassy Te using a machine-learned (ML) interatomic potential to drive molecular-dynamics (MD) simulations of sufficiently large-scale (102,000-atom) glassy Te models for long enough times (>30 ns) to reveal the full chiral-crystallization process [1]. It was discovered that transient cubic-like structural motifs, with lifetimes of only a few ns, act as intermediates in the

creation of chiral crystal-like helical structures from the starting glassy phase, and they also mediate the transfer of chirality between right-hand and left-hand forms, both within chiral-crystal grains and between differently chiral grains at their grain boundaries. The results of related simulations of the melting of crystalline Te will be described, in relation to the operational mechanism of the recently discovered use of Te as an electronic switch for 3D-cross-point non-volatile memory arrays (e.g. of phase-change-memory materials): the off-state of the switch is the semiconducting crystalline state of Te; the on-state is the transient metallic liquid state created by Joule-heating voltage pulses [2, 3]. ML-MD simulations have shown that polycrystalline Te melts at a significantly lower temperature (at grain boundaries) than the single-crystal form, thereby explaining why the first-fire Joule-heating drive voltage is significantly larger than the voltages needed on successive switching cycles [1].

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Nature of Electronic Excitations in Amorphous Phase-Change Memory Materials: $\text{Ge}_2\text{Sb}_2\text{Te}_5$

Konstantinos Konstantinou, University of Turku

Phase-change memory materials based on chalcogenide alloys encode stored digital binary data in the form of metastable structural states. They are strong candidates for neuromorphic and in-memory computing applications, and for next-generation storage-class memory devices. Understanding the nature of electronic excitations is essential for rationalizing the threshold switching and fast crystallization processes of these materials. It is also crucial for addressing the amorphous-phase stability, resistance drift, and reliability issues. In this study, hybrid density-functional theory (DFT) calculations are employed to investigate the lowest triplet excited states in amorphous $\text{Ge}_2\text{Sb}_2\text{Te}_5$. Vertical excitations are modelled with ground-state DFT, followed by relaxation of the triplet excited-state geometry, and subsequent electronic quenching back to the singlet state to assess the structural stability of the glass against electron-hole recombination. In addition, optical excitations in the band gap are examined using linear-response time-dependent DFT, enabling the computation of absorption spectra and excitation energies with hybrid functionals. The results demonstrate the intrinsic formation of self-trapped excitons in amorphous $\text{Ge}_2\text{Sb}_2\text{Te}_5$, and identify the local atomic configurations that can host electron-hole pairs within the glassy network. The simulations provide an atomistic insight into the exciton localization, and the relationship between glass structure and optical properties in chalcogenide phase-change memory materials.

Revisiting the mechanisms of the phase separation and crystal growth by Molecular Dynamics

Lu Deng, Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences

Glass materials have been widely used to meet the demands in various fields, ranging from daily life applications to high technology optics. However, its thermodynamically metastable nature leads to the crystallization becoming a persistent tendency, regardless the length of the time. Although many experimental studies have been performed, understanding at atomistic level is still far from enough. On the other hand, previous simulation studies are also limited

due to various reasons, including un-reliable empirical potentials and unsuitable model construction. In this talk, I will share our recent progresses on phase separation and crystal growth in two different glass systems, i.e., oxyfluoride glass and oxide glass, from the view of molecular dynamics simulations. Fluorine enrichment process during the annealing process and its relationship with temperature will be explored. Moreover, competing mechanisms between crystal growth and melt will be discussed. Furthermore, two observations that are different from classical nucleation theory are investigated. These may provide new atomic insights to the phase separation and crystal growth processes of glass materials.

Identifying the limit of the Tool-Narayanaswamy formalism

Aude Amari, Roskilde University

Physical ageing is a highly non-linear process which indicates gradual modifications in the properties of a system over time due to rearrangement of its particles. The Tool-Narayanaswamy formalism suggests a way to extend the range of applicability of linear response theory by introducing the so-called material time, an internal clock whose ticking rate changes as the system ages [1, 2, 3]. Can this material time always be defined? Is it the same for all ageing quantities? Is it a global or a local clock? We investigate these questions by simulating the physical ageing of a binary Lennard-Jones glass-forming liquid following temperature up-jumps from equilibrated low-temperature states.

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Isomorph Invariance of mechanical properties of model glasses

Nicholas Bailey, Roskilde University

For certain liquids and glass-forming liquids, the potential energy surface has an approximate symmetry which is not obvious from mathematical form of the potential. This approximate symmetry leads to the existence of curves in the phase diagram along which structural and dynamical properties are almost invariant when expressed in appropriate rescaled units. These curves are termed "isomorphs". This property was discovered in simple model liquids including metals, but has also been shown in molecular liquids, and several of its predictions have been verified experimentally. I will present work studying model glasses, using mostly Lennard-Jones potentials, where the invariances have been studied in the context of mechanical properties, specifically dynamical mechanical spectroscopy (DMS) where temperature is varied and the system is sheared at a fixed frequency, as well as Couette shear at fixed strain rate. Identifying the isomorphs, i.e., estimating the appropriate temperature factor for a given density change, is challenging when far from equilibrium. For DMS good invariance is seen. For Couette shear the steady-state properties exhibit excellent isomorph invariance, while the peak stress before entering the flow regime shows distinct deviations from isomorph invariance. These seem to be related to subtleties that emerge when comparing the thermal histories of glasses made at different densities.

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Descriptor-Based and Chemistry-Agnostic Machine Learning Frameworks for Property Prediction and Discovery of Glassy Materials

Suresh Bishnoi, School of Interdisciplinary Research, Indian Institute of Technology Delhi, New Delhi 110016, India

Glasses are archetypal disordered materials for which establishing reliable composition-structure-property relationships remains a central challenge, particularly for emerging non-oxide and functional glass systems. In this work, we present a descriptor-based machine learning framework that combines physically and chemically motivated descriptors to predict optical, mechanical, and thermal properties of glassy materials. The descriptor formulation is designed to encode fundamental atomic and chemical information, enabling transferable models across diverse glass chemistries. The framework is demonstrated using large-scale oxide glass datasets, where descriptor-based models achieve high predictive accuracy while remaining robust across both data-rich and data-sparse regions of the composition space. Model interpretability is enabled through feature-attribution (SHapley Additive exPlanations) analysis, providing insights into how underlying chemical and physical descriptors govern macroscopic glass properties. Importantly, the descriptor formulation enables reliable prediction for glass compositions that do not explicitly appear in the training data, highlighting its chemistry-agnostic and transferable nature. Building on this validated methodology, ongoing and future work aims to extend descriptor-based machine learning strategies to accelerate the discovery of novel glass compositions, including non-oxide and functional glasses, such as high-conductivity glass electrolytes. Overall, this work demonstrates how transferable and interpretable descriptor-based machine learning frameworks can support the rational design of next-generation optical and functional glass materials.

A microkinetic model for describing the molecular scale mechanisms that enhance aluminosilicate glass dissolution

Martin Andersson

Rising CO₂ levels call for quick action. One method for decreasing CO₂ in air and water is mineralisation as carbonate phases. A promising approach is geologic carbon capture and immobilisation in basaltic rocks, such as CarbFix. A key step in the overall process is release of divalent cations. Faster release means faster CO₂ uptake. A dissolution rate quantifies the average rate of release. It is determined from macroscopic experiments, where the effects of many microscopic processes combine to the overall result and is typically empirical. Our aim is to understand the individual, molecular level mechanisms of the macroscopic dissolution rate, where empirical parameters are unnecessary. Organisms produce compounds that enhance basaltic glass dissolution, partly by complexing Al in solution, decreasing dissolved Al activity, promoting further dissolution. However, the effect of organic compound adsorption on solid surfaces has received less attention. Just as organic molecules complex cations in solution, they complex cations on solid surfaces. We studied the dissolution of synthetic calcium aluminium silicate (CAS) and basaltic glass, with and without citrate, in flowthrough dissolution experiments, adsorption studies and with density functional theory (DFT). Our results indicate strong citrate adsorption on glass surfaces, implying that at least some dissolution enhancement results from weakened bonds near the adsorption site. The results input directly to our efforts to develop a microkinetic model that is broadly applicable, for predicting behaviour in mineral-fluid-water-organic compound systems. Gaining such insight contributes to general understanding about what makes organic molecules efficient catalysts in rock weathering and could show the way toward a compound for optimising CO₂ mineralisation.

Structures and structure-property relations of phosphate glasses: insights from atomistic simulations

Jincheng Du, University of North Texas

Phosphate glasses find important technological applications from optics, photonic devices, biomedicine, to nuclear waste disposal. Yet there remain challenges in understanding their atomic structures despite advances obtained from experimental techniques such as diffraction and solid state NMR. In this talk, I will provide an overview of atomistic simulations of phosphate glasses and particularly the efforts in developing effective interatomic potentials for the simulations of these glasses. Our recent effort on developing three-body potentials containing effective partial charge potentials and applications in simulations of binary alkali phosphate, ternary aluminophosphate and iron phosphate glasses will be presented. Recent development of reactive potential to study phosphate glass-water interaction and reactions and examples of studying the phosphate glass-water reactions will be provided.

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Cooling rate effects on CTE of sodium alkaline-earth aluminosilicate glasses

Shingo Urata, AGC Inc.

The coefficient of thermal expansion (CTE) is a critical property for oxide glass when used as a sealing material or carrier substrate, as matching the CTE with that of other materials is essential to prevent deformation, warping, and damage at the interface. The CTE is typically controlled by adjusting the glass composition, while it is also influenced by the cooling rate during the production process. In this study, the CTE and its dependence on cooling rate were experimentally and theoretically investigated for a series of sodium aluminosilicate glasses with the composition $(\text{SiO}_2)_{76-x}(\text{Al}_2\text{O}_3)_x(\text{Na}_2\text{O})_{16}(\text{RO})_8$ ($x = 0 \sim 24$, $R = \text{Ca}, \text{Mg}$). Consequently, the effect of cooling rate was found to be more pronounced in Al_2O_3 -lean glasses, while it was insignificant for glasses with $[\text{Al}_2\text{O}_3] \geq [\text{Na}_2\text{O}]$. To elucidate the mechanism underlying the influence of Al_2O_3 content on the cooling rate dependence of the CTE, molecular dynamics (MD) simulations were conducted using two methods to estimate the CTE. The first method involved heating simulations to evaluate the volume change with temperature, while the second method measured fluctuations in enthalpy and volume to determine the CTE. The effect of cooling rate was investigated by performing MD simulations for two contrasting glass compositions, $x = 0$ and $x = 24$, in $(\text{SiO}_2)_{76-x}(\text{Al}_2\text{O}_3)_x(\text{Na}_2\text{O})_{16}(\text{CaO})_8$. Consequently, the experimental trend was successfully reproduced by both methods when the glass structures were sufficiently equilibrated prior to measuring the CTE. Microstructure analyses revealed that Al_2O_3 doping stabilizes calcium coordination in the glass, thereby reducing the influence of cooling rate on the CTE. This may be attributed to the tendency of alkaline earth ions to localize around aluminum segregation.

Predicting Failure Regions in Sodium Silicate Glasses From its Initial Structure

David Lykkegaard Christensen, Aalborg Universitet

The brittle nature of oxide glasses at macroscale remains its limiting factor causing sudden unanticipated failures that result in reliability concerns, greatly hindering many applications. Therefore, the ability to understand and predict when and how the material fails based solely

on structural information has enormous practical and industrial relevance. Recently deep learning approaches have shown significant promise, successfully learning fractured paths in different atomistic systems, and have been used to study the influence of defects on failure glasses. However, these models have generally been restricted to simple 2D silica systems utilizing Convolutional Neural Network (CNN) models. These are effective for grid-based models, but CNN face fundamental issues when applied to realistic 3D amorphous structure, as they can obscure critical topological information. Therefore, we propose a Graphical Neural Network model with a modified MACE architecture that incorporates a strain-tensor node feature, enabling the model to capture anisotropic details with respect to the loading direction. By integrating this modified MACE architecture with high throughput molecular dynamic fracture simulations of sodium silicate glass structures generated across a range of pressures and compositions show that the machine learning model enables the prediction of fracture propensity across a diverse range of structural and mechanical behaviors. The study provides a framework for predicting the fracture propensity and linking the atomistic structure to the fracture response.

Unraveling the Mixed Glass Former Effect in Sodium Thiophosphate Glass Electrolytes: A Molecular Dynamics Perspective

Alfonso Pedone, University of Modena and Reggio Emilia

The pursuit of safer, cost-effective, and sustainable energy storage systems has directed significant attention toward All-Solid-State Sodium Batteries (ASSSBs). Among the various candidate materials for solid-state electrolytes, amorphous sodium thiophosphate glasses exhibit promising ionic conductivities but face limitations in electrochemical stability. To overcome these drawbacks while preserving favourable transport properties, the Mixed Glass Former Effect (MGFE)—specifically the partial substitution of phosphorus with silicon and sulfur with oxygen—offers a strategic pathway to fine-tune the glass network.[1] In this talk, I will present recent advances in understanding the interplay between composition, atomic structure, and sodium ion conductivity in mixed thiophosphate-silicate and oxy-sulfide glass electrolytes. Using state-of-the-art Machine Learning Interatomic Potentials (MLIPs) trained on first-principles data, we performed extensive Molecular Dynamics simulations to probe how network connectivity, local structural motifs, and modifier distributions impact sodium transport.

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Atomistic Insights into Structure and Dissolution Behaviors of Metal-Organic Framework Glasses for Battery Applications

Tao Du, Harbin Institute of Technology

Emerging metal–organic framework (MOF) glasses have been considered promising electrolyte additive materials for battery applications owing to their isotropic nature, tunable compositions, and adjustable, designable solubility in both organic solvents and aqueous systems. However, the structural dependence of the dissolution behavior of MOF glasses remains underexplored, largely due to their disordered hybrid structures and the non-equilibrium nature of glassy states. In this work, we investigate the disordered structures of MOF glasses and establish the correlation between structural disorder and dissolution behavior using machine-learning-driven atomistic simulations. Our results reveal the structural

origins of MOF glass formation and elucidate how structural disorder modulates dispersion and dissolution behaviors in both organic and aqueous electrolytes. These findings provide new insights for the rational design of advanced electrolyte additives to substantially enhance the performance of batteries.

Establishment of Generalized Empirical Force Fields for Sulfide Glasses and Crystals Used as Superionic Electrolytes in All-Solid-State Batteries

Louis-Martin Poitras, Sorbonne University LPTMC

A generalized Born–Mayer empirical force field has been developed for both crystalline and glassy chalcogenide systems, encompassing sulfide materials containing network formers (e.g., SiS_2 , GeS_2) and alkali or alkaline-earth modifiers (e.g., Li_2S , MgS , CaS). The model integrates fractional charges, short-range Born–Mayer repulsion, long-range dispersion, and harmonic two- and three-body interactions to accurately describe the local structure and connectivity of bridging sulfur atoms between Group III–V polyhedra. Parameterization is achieved through a least-squares minimization against crystallographic data from crystalline phases, further refined by optimizing simulated scattering functions to match experimental X-ray and neutron data for glasses. The resulting force field reproduces key structural features of sulfide glasses, including network depolymerization, Q^n -species distributions, and ring disintegration. Moreover, simulations reveal consistent trends across unreported alkaline-earth thiosilicate and thiogermanate glasses, highlighting similar structural roles of Mg, Ca, and Ba to their alkali counterparts. This transferable and experimentally validated potential opens new perspectives for classical molecular dynamics studies of structural, mechanical, dynamic, and electrochemical properties of disordered sulfide electrolytes and their interfaces, directly relevant to the design of next-generation all-solid-state batteries.

Symposium 1: Fundamentals of glasses: formation, structure and physical properties

Fracture toughness of oxynitride glasses

Theany To, École centrale de Nantes - GeM - CNRS & UnivRennes – IPR

Oxynitride glasses, in which nitrogen replaces oxygen in the glass network, represent a significant advancement in materials science due to their unique structure and superior properties. Compared to oxide glasses, oxynitride glasses exhibit greater chemical durability, hardness, fracture toughness, refractive index, and thermal stability, making them highly promising for structural applications. To examine the influence of nitrogen content on the enhancement of glass properties, we compare the fracture toughness of oxide and oxynitride glasses, measured using the Single-Edge Pre-cracked Beam (SEPB) method. The findings demonstrate that increasing nitrogen content makes the glass stiffer and denser, thereby improving its mechanical properties. Here, by adding 6 at.% of N into an oxide glass, the glass fracture toughness increases to $1.6 \text{ MPa} \cdot \sqrt{\text{m}}$, i.e., by 2.2 times that of the oxide glass.

How to accurately determine the dynamic crack growth exponent for glass materials?

Haizheng Tao, Wuhan University of Technology

The dynamic crack growth parameter n is critical for lifetime prediction of glass materials; however, existing studies suffer from high scatter in reported values due to unstandardized protocols, and the underlying influencing mechanisms remain unclear. To address this issue, this study proposes a standardized evaluation method using soda-lime-silica glass as an example. First, a Weibull statistical model was established to describe the relationship

between Vickers indentation load and crack initiation probability. This allowed the optimal pre-crack load, corresponding to a 100% crack initiation probability, to be scientifically determined, thereby ensuring the consistency of initial flaw conditions. Subsequently, annealing near the glass transition temperature (T_g) was applied, with nanoindentation quantitatively verifying the effective elimination of indentation-induced residual stresses to reveal intrinsic material behavior. On this basis, coaxial ring-on-ring (ROR) tests were performed at varying stress rates ("(" " σ ")"): The characteristic strength (σ_0) was obtained through Weibull statistical analysis, and the n value was determined by linear fitting of the double-logarithmic relationship between $\ln \sigma_0$ and " \ln " " σ " ; achieving a high consistency. This methodology not only significantly reduces experimental uncertainty but also elucidates the roles of pre-crack load and indentation-induced residual stresses in influencing the measured n values, providing a standardized, high-precision, and reproducible approach for characterizing the dynamic fatigue behavior and reliability of glass materials.

In situ mapping of indentation-induced densification and cracking in vitreous silica by nanofocus X-ray scattering

Johan Frederik Schou Christensen, Aalborg University

The practical strength of oxide glasses is greatly reduced by surface flaws that form during processing and use. Instrumented indentation can mimic such real-life damage events and induce flaws and cracking under controlled conditions. At the same time, instrumented indentation allows for systematic examination of the deformation and structural changes of the regions of the glass being indented. However, structural probing is nearly always performed after rather than during the sharp contact event, limiting our understanding of the indentation process. To overcome this, we here demonstrate the use of nanofocus X-ray scattering experiments to probe the local mechanical and structural response of vitreous silica during indentation. Two-dimensional mapping of the scattering pattern in the zone below a sharp diamond wedge indenter reveals local changes in the atomic structure and density as well as cracking behavior. These in situ experiments during indentation reveal the formation and evolution of the densification zone and cracking with nanoscale resolution. Understanding the interplay between structural densification and cracking behavior in glasses is deepened through this work, which is crucial for the development of more damage-resistant and thus stronger glasses as well as fundamental understanding of glass deformation mechanisms.

Impact testing of screen protectors for mobile devices

Anders M. Schade, Aalborg University

The mechanical damage resistance of phone components, particularly screens, is crucial for ensuring the longevity and functionality of modern smartphones. This study investigates the impact resistance of screen protector materials consisting of chemically strengthened glass and thermoplastic polyurethane (TPU) using a developed punch drop test method. The screen protectors were applied to ultra-thin glass (UTG) samples, serving as surrogates for phone screens. The impact resistance was assessed by measuring the average fracture drop height of UTG breakage beneath a screen protector for various punch tip diameters. This outcome was summarised in a parameter termed "protectability". The results indicate that glass screen protectors exhibit superior protection against sharp impacts due to their high stiffness, while the plastic screen protectors provide comparable protection against blunt impacts. Finite element simulations of glass and TPU screen protectors corroborate the experimental findings, highlighting the importance of material stiffness and thickness in enhancing protectability.

Understanding local stress and structural modifications in glass using luminescence of Rare Earth Element and vibrational spectroscopy

Dominique de Ligny, Friedrich Alexander Universität Erlangen-Nürnberg

Although usually considered to be insensitive to their environment, the luminescence of rare earth elements shows significant changes in their emission with pressure and temperature. Their local environment can be modified by elastic or plastic deformation. It is then an unexpected possibility to use them as local structural probes or pressure gauges if appropriate calibration curves are available. In addition, since local changes around rare earth elements differ from larger-scale changes observable by vibrational spectroscopy techniques such as Raman and Brillouin spectroscopy, comparing these different methods can sometimes help distinguish the origin and nature of changes in glass. Here we present the methodology developed by establishing first some calibrations and then applying them to better understand various process-relevant modifications. Experiments using uniaxial press and hot stage allowed the dependencies on pressure and temperature to be determined in the elastic regime. These calibration curves will be finally used to characterize glass under extreme processing conditions such as tempering, aerosol deposition, laser writing or irradiation.

Photo-induced structural dynamics in Ge-Se glasses: a comparative study in the X-ray and visible light range

Stefano Marchesin, Disordered System, DFA Università degli studi di Padova

Chalcogenide glasses show strong photosensitivity over a wide range of wavelengths, including the visible light and the X-ray range. Irradiation induces atomic rearrangements in the glass even far below the glass transition temperature. The germanium-selenide (Ge-Se) family of glasses is a prototypical class of chalcogenide materials whose structure can be finely tuned by varying the relative germanium concentration, leading to significant changes in optical and structural properties. Using X-ray Photon Correlation Spectroscopy (XPCS) we investigated different Ge(x)-Se(1-x) compositions ($x = 10, 20, 25$) at room temperature to study the photo-induced dynamics as a function of the X-ray dose rate. We then compared this dataset to viscosity measurements of Ge-Se fibers with the same composition irradiated using sub-bandgap visible light. We find that, despite the large differences in photon energy and dose rates, the photo-induced dynamics under visible and X-ray irradiation follow a similar trend, indicating similar irradiation-driven structural rearrangements. These results help to elucidate the still not fully understood mechanisms underlying photo-induced defect creation in chalcogenide glasses.

Invert glasses of high optical basicity

Doris Möncke, Inamori School of Engineering, New York State College of Ceramics at Alfred University

Invert glasses, oxide glasses that contain a higher fraction of modifier oxide than network former oxide, are per definition high basicity glasses, as the polarizability of classical network former is much lower than that of modifier oxides. Invert glasses lack a three-dimensional network based on network former polyhedra that are linked via directed covalent bonds; instead, cations and polyanions such as ortho units, anions of network former such as $(\text{SiO}_4)^{4-}$, $(\text{BO}_3)^{3-}$ or $(\text{PO}_3)^{-}$, and pyro units, dimers like $(\text{Si}_2\text{O}_7)^{6-}$, $(\text{P}_2\text{O}_7)^{4-}$, $(\text{B}_2\text{O}_5)^{4-}$. For borates, tetrahedral borate units with non-bridging oxygen might also be present. Such glasses will be discussed in view of bonding ionicity, optical basicity, structure and properties. For example, invert glasses of high optical basicity are known to stabilize unusually high oxidation states of transition metal ions, such as Co^{3+} , Ni^{3+} or even Mn^{5+} and Mn^{6+} . High basicity glasses can also stabilize unusual oxo-anions such as $(\text{SO}_4)^{2-}$, $(\text{NO}_3)^{-}$ or $(\text{CO}_3)^{2-}$ and might also contain chemically dissolved oxygen not bonded to classical network former. I prefer to reserve the

term “free” oxygen for physically dissolved molecular oxygen or oxygen radicals, but oxide ions that connect only to modifier cations are a significant species, not only in sub-ortho compositions. The concentration of chemically dissolved oxygen seems to increase with the cation field strength and the amount of modifier oxides. Furthermore, the higher the cation’s field strength, the lower is the ionicity of the cation-oxygen bonds, so that the traditional classification into modifier and network former can be lost, e.g. when melting “pure” Bi₂O₃ in a fire clay crucible. Here, dissolution of the crucible provides enough impurities to allow glass formation. Since invert glasses are often very corrosive, crucible melt interactions cannot be ignored. Invert glasses with cations of higher field strength can be very stable.

Insights into the Structure-Property Relationships and Conduction Mechanisms in Glassy Sulfide Electrolytes

Louis-Martin Poitras, Sorbonne University LPTMC

Understanding the relationship between atomic structure and ion transport is essential for advancing glassy sulfide electrolytes as next-generation solid-state battery materials. This work investigates how local structural motifs, network connectivity, and modifier concentration govern mechanical stability and ionic conductivity in sulfide glasses. Classical molecular dynamics simulations are employed to probe the influence of composition and temperature on the microscopic conduction mechanisms, including ion migration pathways and their correlation with network depolymerization and Qⁿ-species distributions. Preliminary analyses reveal trends linking structural disorder to enhanced mobility and mechanical response, offering an atomistic perspective consistent with experimental observations. This study provides a unified framework for exploring the interplay between structure, dynamics, and transport in sulfide glass electrolytes, paving the way for rational design of solid-state battery materials with optimized performance and stability.

New sodium-conducting glass compositions obtained by mechanochemistry: synthesis, structure, and properties

Louisiane Verger, University of Rennes, CNRS

Sulfur-based glasses are attracting growing interest as solid-state electrolytes because of their high ionic conductivity compared to their oxide counterparts, and their mechanical properties. They are classically synthesized by the melt quenching method in silica tube. However, this process poses problems of safety, scalability, cost and limits the glass compositions available, due to the reactivity of alkali with silica. An alternative to high-temperature syntheses and solvent-based processes is the use of mechanical milling techniques. In this talk, we show how mechanochemistry can be used to extend the glass forming domain in the Na₂S-Ga₂S₃ pseudo binary and the Na₂S-Ga₂S₃-GeS₂ pseudo ternary. The influence of the addition of selenium (Se) on the glass formation will also be discussed. The conductivity properties and structure of these new Na and Ga-rich glasses are discussed, based on high-field solid-state nuclear magnetic resonance spectroscopy (²³Na and ⁷¹Ga) as well as by X-ray total scattering and pair distribution function analysis.

Role of organic linkers in controlling the deformation and fracture behavior of cyano-functionalized zeolitic imidazolate frameworks

Xiaoyi Xu, Aalborg University

Zeolitic imidazolate frameworks (ZIFs) are a subclass of metal–organic frameworks with high structural flexibility, which is beneficial for many applications, but also makes their mechanical behavior difficult to control. Cyano functionalization has been shown to influence the thermal behavior and glass-forming ability of ZIF-4, yet its effect on mechanical response is still not

well understood. In this work, we use molecular dynamics simulations based on a machine-learned force field to investigate how cyano groups modify the deformation and fracture behavior of ZIF-4 in both crystalline and glassy states. We find that pristine ZIF-4 accommodates tensile strain primarily through a hinge-like torsional rotation of the Zn–imidazole–Zn units, allowing significant flexibility before bond breaking occurs. With cyano substitution, this torsional motion is suppressed, leading to increased rigidity of the hinge and a shift in the deformation mechanism toward Zn–N bond stretching. Interestingly, this torsion-to-stretching transition is also observed in the glassy phase, suggesting that the effect of cyano functionalization is largely independent of structural order. Additional analysis suggests that the electron-withdrawing nature of the cyano group modifies the electronic distribution in the linker, which may contribute to the reduced rotational flexibility.

Reticulating node-linker-strut chemical spaces for metal-organic network-forming glasses by synergistically promoting configurational degree of freedoms

Yingbo Zhao, ShanghaiTech University

Hybrid glasses with metal-organic composition are emerging type of network-forming glasses that combines the modulator designability of MOFs and the processability of glasses. However, the melt-quenching method is not applicable to most crystalline MOFs due to thermal decomposition before melting. Consequently, the number of known glassy MOFs are very limited compared to the vast library of crystalline MOFs and CPs. Such limitation fundamentally originates from the lack of degree-of-freedom for these crystalline MOFs, which are necessary for generating the collective motions in glass transition. To mitigate such limitation and establish rich chemical space for glassy coordinative networks, we have developed systematic methods to promote dynamics in these networks: (a) employing metal nodes with multiple coordinative sites or coordination geometries; (b) installing flexible motifs to the organic linker; (c) using coordinative modulator to decrease the network connectivity. Using such methodology, we achieved modular synthesis of metal-alkoxide network-forming glasses made from a variety of metal-oxo clusters (including Ti, Zr, Al) linked with alcohol linkers that can be synthesized at low temperature with environmentally friendly solvent. Glasses made from aluminum-oxo clusters linked with alcohol linkers shows optical transparency and tunable microporosity up to 500 m²/g with well-defined glass transition temperature before activation. We also elucidate the mechanism of their synthesis in several model systems by combining rheology, differential scanning calorimetry and pair-distribution functions, which shows the evaporation of coordinatively competitive solvents leads to increased network connectivity and relaxation time, which ultimately lead to vitrification. This strategy is also used to vitrify prototype MOFs with rigid aromatic dicarboxylate linkers such as MOF-5 and MIL-101, producing a series of glasses with tunable properties controlled by modulator content and metal compositions.

Hybrid Glass Formation in Coordination Polymers via Aliphatic Chain Dynamics

Minhyuk Kim, Ewha Womans University

Hybrid glasses derived from coordination polymers (CPs) promise a fusion of processability and structural functionality, yet their formation is fundamentally limited by poor thermal stability and high melting points. Here, we demonstrate a mesophase-mediated vitrification mechanism in a series of magnesium-based CPs (MgC_nDC, n = 2–7) featuring aliphatic dicarboxylate linkers. Upon thermal desolvation, these frameworks transition into a mesomorphic state that retains long-range order and coordination integrity while inducing conformational disorder within the organic substructure. This intermediate state enables a direct glass transition without requiring full melting. The resulting glasses exhibit distinct calorimetric transitions and tunable mechanical properties governed by chain length. Furthermore, only the longest-chain analogue (n = 7) undergoes conventional melting, yielding

a melt-quenched glass with lower mechanical stiffness due to the partial dissociation of its metal-organic backbone. Spectroscopic and structural analyses reveal that mesophase vitrification proceeds via unlocking rotational freedom in the methylene chains, drawing strong parallels to semicrystalline polymer behaviour. These findings establish a design strategy for vitrifiable coordination networks by integrating principles from polymer dynamics and mesomorphism.

Generic Vitrification of Prototype Metal-Organic Frameworks Linked by Rigid Dicarboxylate Linkers

Meihua Qin, ShanghaiTech University

Vitrifying crystalline metal-organic frameworks (MOFs) is an emerging route to creating processable, glassy materials with novel functions. However, a vast portion of MOFs, such as the seminal MOF-5, are constructed from rigid aromatic dicarboxylate linkers. While essential for reticular design, these aromatic dicarboxylate linkers impart low configurational entropy, which has historically precluded the vitrification of a major portion of MOFs. Here, we report a generalizable strategy to overcome this limitation by synergistically promoting configurational degree of freedom, which combines grafting flexible side chains onto the rigid linkers, employing mixed-metal nodes, and introducing coordination modulators to tune network connectivity. This strategy is demonstrated by successfully vitrifying functionalized MOF-5 and MIL-101, producing a series of glasses with tunable properties controlled by modulator content and metal composition. The resulting glasses exhibit promising functional properties, including high photoluminescence quantum yields, uniformity and robustness as host matrix for optically pumped laser. This work establishes rational design principles for converting rigid MOFs into glassy materials, unlocking a vast library of reticular structures for the development of new functional glasses.

Poster abstracts

Effect of Hydrothermal Treatment on Surface Chemistry, Tribology, and Crack Resistance of Alkali Boroaluminosilicate Glasses

Elsebeth Juhl Pedersen, Department of Chemistry and Bioscience, Aalborg University, 9220 Aalborg, Denmark

It is well-known that water can lead to stress corrosion in glasses, but certain glass compositions can show an improvement in crack initiation resistance upon hydrothermal treatment, e.g., upon treatment of various multicomponent silicate glasses with water vapor at elevated temperature. Here, we study the effect of such hydrothermal treatment on the surface chemistry of two series of alkali-boroaluminosilicate and alkali-aluminosilicate glasses. Through indentation, friction/wear, NMR, XPS and infrared to ultraviolet spectroscopic ellipsometry measurements, we determine the changes in mechanical properties, surface structure and surface chemistry. These insights contribute to a deeper understanding of the mechanism behind the water vapor induced strengthening in complex glass systems. By elucidating the interplay between surface chemistry and mechanical performance, our study lays the groundwork for tailoring hydrothermal treatments to enhance glass mechanics.

Li-Ion Transport and Mechanics of Li-S-P-B-I Glassy Electrolytes

Yong Li, Aalborg University

Glassy sulfide and halide-based electrolytes are promising candidates for all-solid-state lithium batteries owing to their high ionic conductivity and good processability. Their ionic transport and mechanical properties depend on the complex local structure, but structure-property relations are not yet fully understood. This work employs molecular dynamics simulations with a machine learning force field (MLFF) to reveal how the competition between flexible B-S and rigid P-S networks govern the properties of Li-S-P-B-I (LSPBI) glasses across a full composition range (0P₂S₅ to 100P₂S₅). The developed MLFF accurately reproduces ab initio reference data and enables large-scale simulations to explore dynamics and mechanics mechanisms. The distinct roles of B-S and P-S bonding networks govern both ionic transport and mechanical response in the glassy Li-S-P-B-I electrolytes. B-S bonds tend to form more flexible and reconfigurable local structures, which facilitate Li-ion migration through transient bond rearrangements. In contrast, the stronger and more directional P-S bonds generate a rigid network that suppresses Li mobility but enhances mechanical stiffness. Under external stimuli, the out-of-equilibrium interactions between Li and its S-coordinated neighbors promote local bond-switching events in B-S environments, while P-S frameworks resist such rearrangements. This compositional contrast explains the simultaneous variation of ionic conductivity and fracture resistance as the relative proportions of B-S and P-S units evolve. This work provides atomistic insight into how chemical composition governs transport and mechanical properties in Li-S-P-B-I glass electrolytes, offering guidance for the design of robust and high-performance solid electrolytes.

Optical and Scintillation Properties of Ce-doped KGd(PO₃)₄ Metaphosphate Glasses

Daiki Shiratori, Tokyo University of Science

A scintillator is a luminescent material that promptly converts ionizing radiation into visible photons and is indispensable for technologies based on radiation detection. Most scintillators currently in practical use are single crystals; however, compared with other materials, single crystals are often industrially inconvenient because their fabrication cost is high, and shaping into large or complex geometries is difficult. In contrast, glass materials offer excellent formability and relatively low production cost, making them effective for certain applications. A major drawback is that glass scintillators generally exhibit light yields markedly lower than those of crystals. To address this issue, we have been investigating metaphosphate glass

systems. In particular, we have considered Ce-doped NaGd(PO₃)₄ glass as a promising candidate. Our results suggest that Gd-to-Ce energy transfer can compensate for poor energy-transport efficiency in glass scintillators, leading to a high light yield of ~1900 ph/MeV. In the present study, aiming to improve X-/γ-ray absorption (stopping power) by increasing the effective atomic number, we focused on KGd(PO₃)₄ glass with Na substituted by K. Ce-doped KGd(PO₃)₄ glasses were synthesized by the conventional melt-quenching method, and their optical and scintillation properties were measured. The scintillation spectra showed distinct emission attributable to the Ce³⁺ 5d–4f transition. From pulse-height spectra measured with 662 keV γ-rays from a ¹³⁷Cs source, the light yield was estimated to be ~2000 ph/MeV. In this presentation, we will introduce the detailed optical and scintillation characteristics of Ce:KGd(PO₃)₄ glasses.

Chemical modification of zeolitic imidazolate framework glass electrolytes

Søren Clement Juhl Hansen, Aalborg Universitet

Solid-state batteries with a metal anode offer an improved energy density and safety compared to batteries based on flammable liquid electrolytes. To this end, metal-organic framework (MOF) glasses show promising potential as solid state electrolytes due to their isotropic, grain boundary-free conduction and thermal stability. The main focus of this work is to enhance Li-ion conductivity in MOF glass electrolytes, specifically ZIF-62, through electronic and compositional modification of the organic linkers. The aim is to obtain materials with a room temperature ionic conductivity above 10⁻³ S cm⁻¹. First, co-melting ZIF-62 crystals with modifying agents is employed to alter the electronic and compositional motifs. Initial modification uses benzimidazolium chloride (H₂Bim-Cl) to significantly lower the melting temperature to below 300 °C and electronically engineer the Zn²⁺ nodes. Molecular simulations suggest that the introduced halide anions partially replace imidazolate linkers, increasing the fraction of undercoordinated Zn sites. Second, lithium benzimidazolate (LiBim) is utilized as a modifier, incorporating Li⁺ into the MOF glass structure itself. The final dense, isotropic ZIF-62 glass structure is further expected to enhanced electrochemical stability (up to 5 V) and mechanically suppress Li dendrite penetration, ensuring excellent long-term cycling performance.

Understanding the Effect of Na₂O and B₂O₃ content on Intermediate Sodium-Aluminoborosilicate Glasses with Self-Terminating Crack-Loop

David Lykkegaard Christensen, Aalborg Universitet

Sodium-aluminoborosilicate glasses (Fusion5) are promising alternatives to other brittle oxide glasses due to their mechanical properties and the distinct formation of a self-terminating crack loop that bounds and hinders the propagation of strength-limiting radial and lateral cracks during Vickers indentation. These types of glass exhibit an intermediate deformation response between that of highly densifying (anomalous, e.g., pure silica) and highly shear-flowing (normal, e.g., soda-lime-silica) glasses. However, little is known about the controlling factors of self-terminating cracking. In this study, the relationship between chemical composition, deformation mechanism, and self-terminating crack behavior is investigated for glasses with compositions of xNa₂O-(100-x)[14.03B₂O₃-4.64Al₂O₃-81.33SiO₂] (x = 6.5-21.5) and xB₂O₃-(100-x)[10.88Na₂O-4.81 Al₂O₃-84.31SiO₂] (x = 0-31). Indentation experiments reveal that the formation of ring cracks is highly sensitive to changes in Na₂O, while exhibiting surprisingly little to no dependence on B₂O₃. Notably, the self-terminating crack loops are even found in compositionally simple systems of Na₂O-Al₂O₃-SiO₂. The results further show that self-terminating crack formation is only partially dependent on the relative contributions of shear flow and densification during deformation and that this does not directly dictate the self-terminating crack pattern. Overall, the findings highlight the alkali content as the dominant factor that governs self-terminating crack behavior.

Fracture toughness of calcium aluminosilicate glasses

Sidsel Mulvad Johansen, Department of Chemistry and Bioscience, Aalborg University, 9220 Aalborg East, Denmark

A major limitation of oxide glasses is their low fracture toughness, leading to premature failure as a result of critical flaws. A thorough understanding of how fracture toughness is linked to the glass composition and structure still needs to be developed. Here, we investigate the fracture toughness of the important family of calcium aluminosilicate glasses by means of the Single-Edge Precracked Beam (SEPB) method. We connect the glass structure to the fracture toughness by investigating glasses with varying silica contents and alumina/calcia ratios, encapsulating both percalcic and peraluminous compositions. By molecular dynamics simulations, validated by X-ray total scattering, we correlated the fracture toughness to specific structure features. We infer that local coordination changes of aluminum, so-called bond switching, correlate positively with the fracture toughness. We further extend our investigation to include hardness, crack initiation resistance and elastic moduli, finding that various structural features should be considered to understand each of these mechanical properties within the calcium aluminosilicate glass family.

Ultra-thin Glass with Low Young's Modulus for Foldable Display

Jinwook Jang, Department of Advanced Materials Engineering, Kongju National University, Republic of Korea

Recent expansion of foldable electronics market spurred the demand for flexible transparent substrates such as ultra-thin glass (UTG). Sodium aluminosilicate (SAN) glass is commonly used for UTGs thanks to its high robustness and resilience after chemical strengthening. However, its brittle characteristics which induce cracks, breakages and other field failures still remain to be solved. Previous studies have reported that SAN glass exhibits excellent ion-exchange performance for chemical strengthening when the $\text{Al}_2\text{O}_3/\text{Na}_2\text{O}$ ratio is fixed at 1, and the glass needs low Young's modulus for the enhanced flexibility. In this study, a super-flexible and ion-exchangeable glass for foldable displays is introduced by reducing the Young's modulus of the glass. Young's modulus was effectively reduced from 72 to 53 GPa by substituting SiO_2 with B_2O_3 and P_2O_5 while maintaining the $\text{Al}_2\text{O}_3/\text{Na}_2\text{O}$ ratio at 1. The bending characteristics of the glasses were evaluated using indentation and two-point bending tests. The resulting low-modulus glasses exhibited enhanced flexibility, characterized by high fracture toughness, superior resistance to flaw formation, and reduced bending repulsive force—attributes that imply a smaller folding radius. This flexibility, which enables the glass ideal for foldable device applications, is discussed in terms of structural change induced by composition as evidenced by solid-state NMR and Raman spectroscopy.

Photoluminescence and thermoluminescence properties of Tl-doped magnesium aluminoborate glasses for radiation dosimetry

Shota Otake, Nara Institute of Science and Technology

Phosphor-based dosimeters are widely used in fields such as environmental monitoring, personal dosimetry, and medical imaging. These devices employ storage phosphors, whose luminescence intensity depends on the accumulated radiation dose. In particular, for applications in personal dosimetry, it is important that the materials exhibit high detection sensitivity in the low-dose region, good linearity of luminescence intensity with respect to the absorbed dose, low fading characteristics, and a low effective atomic number (Z_{eff}) to ensure tissue equivalence. In this study, Tl-doped $\text{MgO-Al}_2\text{O}_3\text{-B}_2\text{O}_3$ (MAB) glass was prepared as a novel storage phosphor material, and its luminescence properties were systematically evaluated. MAB glass possesses excellent chemical stability as well as a Z_{eff} close to that of human tissue. Previously, MAB glasses doped with Sn, Ce, and Tb have been reported to exhibit good detection sensitivity over a wide dose range. Tl is known to exhibit highly efficient luminescence based on s-p transitions in the blue-to-green spectral region, where

conventional photodetectors show high sensitivity, and Tl-doped phosphors such as Tl:NaI and Tl:Csl have been widely used in the field of radiation detection. In this work, Tl:MAB glass samples with different Tl concentrations were prepared using the melt-quenching method. The fabricated samples exhibited a broad emission band attributed to Tl⁺ in the wavelength range of 300–400 nm, and the highest photoluminescence quantum efficiency was obtained for the 0.1% Tl-doped sample. Furthermore, thermoluminescence glow curve measurements of the Tl:MAB samples revealed a luminescence peak located at approximately 200 °C. In addition to the Tl concentration dependence of these results, detailed luminescence characteristics, such as dose response and fading behavior, will also be discussed at the conference.

Ionizing-radiation induced luminescence properties of Eu-doped SrO-Al₂O₃ glasses

Daisuke Nakauchi, Nara Institute of Science and Technology

Scintillators are a class of phosphors that emit light upon excitation by ionizing radiation. They are widely utilized in fields such as medical imaging and security because of their ability to immediately convert high-energy radiation (keV-GeV) into tens of thousands of photons. Eu-doped alkaline-earth metal compounds have long been recognized as high-performance phosphors. Specifically, Eu-doped SrAl₂O₄ has been extensively studied in the field of persistent phosphors. Although its application as a scintillator was previously limited, recent studies have revealed that Eu-doped SrAl₂O₄ single crystals exhibit a high scintillation light yield of 46,000 ph/MeV. While single crystals are the conventional form for scintillator materials, they face challenges regarding production costs and shape flexibility. Conversely, glass scintillators—except for 6Li-glass—have not been widely commercialized despite their superior manufacturability. Hypothesizing that the SrO–Al₂O₃ system could maintain high scintillation performance even in a glassy state, we synthesized Eu-doped SrO–Al₂O₃ glasses using the containerless processing method with an aerodynamic levitation furnace. In this study, we evaluated the photoluminescence and radioluminescence properties of the resulting glasses to assess their potential for radiation detection applications.

Indenting glasses with indenters of varying stiffness and sharpness

Johan Frederik Schou Christensen, Aalborg University

The instrumented indentation technique is widely used to evaluate the mechanical properties of glasses. This is due to its versatility and ability to evaluate several properties, while it is still a relatively simple technique that is reasonably easy to employ. A pivotal aspect of the design of indentation experiments is the properties of the indenter, i.e., the object pressed into the glass. However, systematic knowledge of how the indenter properties affect the indentation response is scarce. To address this, we have systematically examined the indentation response of three oxide glasses (sodium silicate, sodium borate, and sodium borosilicate) while varying the indenter sharpness and the indenter material, thus the indenter stiffness. We observe decreasing indenter sharpness to favor densification relative to shear flow deformation, which in turn is correlated to a lower propensity for crack initiation. The indenter sharpness does not affect the measured hardness of the glasses at relatively high loads, yet sharper indenters reduce the magnitude of the indentation size effect, which affects hardness measurements at low loads. We find the indenter stiffness to affect the indentation response when the stiffness is of similar magnitude to that of the glass under examination, as this causes significant elastic deformation of the indenter itself, while stiffer indenters can be considered rigid. This deformation of a less stiff indenter is found to reduce its effective sharpness. Our findings are useful for guiding the design of indentation experiments in terms of indenter properties, while also providing new insights into the indentation response of oxide glasses regarding crack initiation and the indentation size effect. The obtained knowledge is also relevant for the use of the instrumented indentation technique to evaluate the real-life resistance of glasses to contact damage, as the use of non-conventional indenters might be more appropriate for mimicking real-life contact events.

Optical and X-ray induced luminescence properties of $x\text{TbF}_3\text{-(30-x)}\text{SrF}_2\text{-20Al}_2\text{O}_3\text{-50B}_2\text{O}_3$ glasses

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Scintillators are a type of optical material that immediately converts the absorbed energy of ionizing radiation into low-energy photons. A typical scintillation detector consists of a scintillator combined with a photodetector. Recently, K. Shinozaki et al. reported that oxyfluoride glasses such as $\text{AEF}_2\text{-Al}_2\text{O}_3\text{-B}_2\text{O}_3$ (AE = Mg, Ca, Sr, Ba) exhibit high quantum yields. In general, glass materials offer advantages over single crystals, including lower cost and easier fabrication. In this study, $x\text{TbF}_3\text{-(30-x)}\text{SrF}_2\text{-20Al}_2\text{O}_3\text{-50B}_2\text{O}_3$ ($x = 0.1\text{--}20$ mol%) glasses were investigated, and their optical and X-ray-induced luminescence properties were evaluated. The 10%Tb-doped glass exhibited sharp emission peaks in the range of 480–630 nm under excitation at 340–380 nm, showing the highest quantum yield of approximately 100%. The photoluminescence decay curve was well fitted by a single exponential function, with a lifetime of 2.7 ms, which is typical for the 4f–4f transitions of Tb^{3+} ions. Under X-ray irradiation, the same emission was also observed, demonstrating the potential applicability of oxyfluoride glasses for X-ray detector applications.

Atomistic Transitions in Intermediate Calcium Aluminoborosilicate Glasses under Indentation

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Enhancing the damage resistance of glass surfaces is crucial for extending service lifetimes and preserving the aesthetics of numerous products, ranging from smartphone screens to architectural elements. By and large, surface damage arising from physical contact, such as indentation and cracking, contributes significantly to the mechanical weakening of glass components, necessitating the investigation of the forerunning deformation mechanisms. In this study, we explore the atomic-scale indentation deformation of a family of intermediate calcium aluminoborosilicate glasses using the molecular dynamics method. A rigid diamond indenter is driven into the glass surface, followed by a detailed topographic analysis of surface pile-up and sink-in behavior. In particular, the relative extents of densification (network compaction) and shear flow (bond reconstruction) modes are examined during indentation. Further, the short- and medium-range structural features attributing to the deformation modes are evaluated to establish direct correspondence with experimental observations. In summary, the simulations reveal the atomic-scale structural transitions governing indentation deformation in intermediate oxide glasses and provide mechanistic insights into enhancing their damage resistance.

Establishment of Generalized Empirical Force Fields for Sulfide Glasses and Crystals Used as Superionic Electrolytes in All-Solid-State Batteries

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A generalized Born–Mayer empirical force field has been developed for both crystalline and glassy chalcogenide systems, encompassing sulfide materials containing network formers (e.g., SiS_2 , GeS_2) and alkali or alkaline-earth modifiers (e.g., Li_2S , MgS , CaS). The model integrates fractional charges, short-range Born–Mayer repulsion, long-range dispersion, and harmonic two- and three-body interactions to accurately describe the local structure and connectivity of bridging sulfur atoms between Group III–V polyhedra. Parameterization is achieved through a least-squares minimization against crystallographic data from crystalline phases, further refined by optimizing simulated scattering functions to match experimental X-ray and neutron data for glasses. The resulting force field reproduces key structural features of sulfide glasses, including network depolymerization, Q^n -species distributions, and ring disintegration. Moreover, simulations reveal consistent trends across unreported alkaline-earth thiosilicate and thiogermanate glasses, highlighting similar structural roles of Mg, Ca, and Ba to their alkali counterparts. This transferable and experimentally validated potential

opens new perspectives for classical molecular dynamics studies of structural, mechanical, dynamic, and electrochemical properties of disordered sulfide electrolytes and their interfaces, directly relevant to the design of next-generation all-solid-state batteries.

Radio-photoluminescence characteristics in Au-doped sodium aluminophosphate glass

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Radio-photoluminescence (RPL) is a phenomenon in which electrons and holes generated by ionizing radiation form new luminescence centers, which then emit light upon excitation. Since RPL intensity can be proportional to the absorbed radiation dose, RPL materials are applicable for radiation dosimetry. The common RPL material is Ag-doped sodium aluminophosphate glass. This material exhibits excellent RPL properties. To further improve the RPL properties and reveal the fundamental RPL phenomena, many novel materials have been investigated in their RPL properties. In this study, Au-doped sodium aluminophosphate glass was synthesized by the conventional melt quenching method, and the photoluminescence (PL) and RPL properties were investigated. The broad luminescence peak was observed at around 800 nm under the excitation wavelength at around 340 nm. The origin of luminescence at around 800 nm was attributed to the Au dimer (Au₂⁺) or trimer (Au₃⁺). The RPL intensity monotonically increased with increasing irradiation dose from 10 to 100 Gy. The RPL intensity after 100 Gy irradiation was measured at 10-minute intervals for 60 minutes. The RPL intensity was stable during the measurement. The result revealed that the newly generated RPL centers were stable against the excitation light. The stability of the luminescence center offers significant advantages when using it as a personal radiation dosimeter. The stability of the RPL intensity against heat was also investigated. When the Au-doped glass sample was annealed until 150 °C for 10 minutes, the RPL spectra were almost the same as that of at room temperature. In contrast, the RPL peak at ~800 nm disappeared when the annealing temperature was over 200 °C. These results revealed that the RPL intensity was stable against the excitation light and heat at around room temperature.

Fracture toughness of zeolitic imidazolate framework crystal–glass composites revealed by molecular dynamics simulations

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Zeolitic imidazolate framework (ZIF) glasses are attractive for applications such as energy storage and gas separation, yet their limited fracture toughness restricts practical deployment. In this work, we employ molecular dynamics simulations with machine learning force fields to design and evaluate ZIF crystal–glass composites. The composites comprise ZIF-4 or ZIF-zni crystalline domains embedded in a melt-quenched ZIF-4 glass matrix. ZIF-4 and ZIF-zni share the same chemical composition (ZnIm₂, Im = imidazolate) but differ in density and stiffness, with ZIF-zni exhibiting a significantly denser crystal network. Composites containing the stiffer ZIF-zni crystals show a pronounced improvement in fracture resistance, as crack propagation is hindered by irreversible atomic rearrangements and deflected around the crystalline domains. Moreover, the morphology of the inclusions plays a crucial role: round-shaped domains are particularly effective in guiding crack deflection and preserving structural integrity in the elastic regime. Atomic-scale analysis further identifies a structural factor that governs stress distribution and fracture response in the composites. These findings provide fundamental insights into the fracture mechanisms of ZIF-based hybrid glasses and establish a design strategy for engineering metal–organic framework composites with enhanced mechanical reliability.

Indentation behavior of alkali aluminoborosilicate glasses

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Glasses are utilized in everything from phone screens to windshields. Despite this versatility, their primary limitation remains their susceptibility to cracking, leading to failure. This vulnerability is characterized through indentation experiments, where normal glass undergoes shear flow, typically leading to radial and lateral cracks, while anomalous glasses densify, typically creating cone cracks around the indent periphery. Recent studies on “intermediate” glasses, specifically some sodium aluminoborosilicate glasses, have found a new type of crack morphology, namely a ring crack around the impact area with radial cracks running from the impact site to said ring. This cracking behavior has been linked to deformation through a larger amount of densification compared to normal glasses, while having higher shear flow than anomalous glasses. However, the specific mechanisms and glass composition and structure resulting in this indentation behavior remain poorly understood. This study investigates these mechanisms by varying the alumina content and type of alkali species, i.e., replacing sodium with lithium, potassium, or rubidium. The aim is to elucidate the mechanisms behind this cracking behavior and assess these glasses’ mechanical properties.

Optical properties of the $\text{PbCl}_2\text{-BiO}_3/2\text{-TeO}_2$ glasses doped with Er^{3+} and $\text{Er}^{3+}/\text{Yb}^{3+}$

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This study investigates the photoluminescence behaviour of $\text{PbCl}_2\text{-BiO}_3/2\text{-TeO}_2$ glasses doped with Er^{3+} and $\text{Er}^{3+}/\text{Yb}^{3+}$ ions, with emphasis on their suitability for temperature sensing applications. Under 514.5 nm excitation, the visible emission spectra are dominated by two green bands centred at 526 and 550 nm, accompanied by a weaker red band around 660 nm. In the near infrared region, the strongest emission occurs at 1530 nm, corresponding to the $^4I_{13/2} \rightarrow ^4I_{15/2}$ transition of Er^{3+} , while two much weaker bands appear near 860 and 1230 nm. All observed 4f–4f transitions exhibit a linear dependence of integrated luminescence intensity on Er^{3+} concentration, indicating the absence of concentration quenching within the investigated range. Efficient up conversion luminescence is detected under 980 nm excitation, producing green, red, and near infrared bands typical of multi photon Er^{3+} processes. The influence of Yb^{3+} co doping is examined for both up conversion and downshifting luminescence, revealing enhanced emission efficiency due to Yb^{3+} sensitised energy transfer. In Yb^{3+} containing glasses, an intense emission band appears around 900 nm under 980 nm excitation, consistent with efficient $\text{Yb}^{3+} \rightarrow \text{Er}^{3+}$ energy transfer pathways. The relative intensities of the emission bands, particularly the red to green ratio, demonstrate strong temperature sensitivity, confirming that both downshifting and up conversion emission processes can be exploited for optical thermometry. These findings highlight Er^{3+} and $\text{Er}^{3+}/\text{Yb}^{3+}$ doped $\text{PbCl}_2\text{-BiO}_3/2\text{-TeO}_2$ glasses as promising materials for luminescence based temperature sensing across the visible and near infrared spectral regions. The work was supported by the Czech Science Foundation [Grant No. 25-15635S].

Spectroscopic Characterisation of Rare Earth Doped Oxychloride Tellurite Glasses Containing Pb and Bi

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An overview is provided of the optical and photoluminescence behaviour of 20 $\text{PbCl}_2 - 10 \text{BiO}_3/2 - 70 \text{TeO}_2$ glasses doped with Er^{3+} , $\text{Er}^{3+}/\text{Yb}^{3+}$, and Ho^{3+} ions. The glasses are shown to exhibit broad transparency extending into the near infrared together with high refractive index, enabling efficient excitation and emission across visible and NIR regions. Upon RE doping, characteristic downshifting luminescence arising from 4f–4f transitions is observed, and up conversion processes are detected in samples containing Er^{3+} and $\text{Er}^{3+}/\text{Yb}^{3+}$. In Er^{3+} doped glasses, green and red emissions are recorded together with a dominant band near 1530 nm, accompanied by weaker NIR transitions. When co doped with Yb^{3+} , a substantial enhancement of both downshifting and up conversion luminescence is obtained due to $\text{Yb}^{3+} \rightarrow \text{Er}^{3+}$ energy transfer, including the appearance of an intense emission near 900 nm under

980 nm excitation. In Ho^{3+} doped samples, the expected green and near infrared emissions associated with Ho^{3+} multiplet transitions are identified. Across all RE doped compositions, photoluminescence intensities are found to vary systematically with dopant concentration. Lifetime measurements of the relevant excited states are included alongside the spectral data to provide complementary insight into radiative and non-radiative relaxation pathways. Overall, the results indicate that RE doped $\text{PbCl}_2\text{-BiO}_3/2\text{-TeO}_2$ glasses form a versatile platform for visible and near infrared photonic applications, offering strong downshifting emission and tunable up conversion responses suitable for sensing and related optical technologies. An overview is provided of the optical and photoluminescence behaviour of 20 $\text{PbCl}_2 - 10 \text{BiO}_3/2 - 70 \text{TeO}_2$ glasses doped with Er^{3+} , $\text{Er}^{3+}/\text{Yb}^{3+}$, and Ho^{3+} ions. The glasses are shown to exhibit broad transparency extending into the near infrared together with high refractive index, enabling efficient excitation and emission across visible and NIR regions. Upon RE doping, characteristic downshifting luminescence arising from 4f-4f transitions is observed, and up conversion processes are detected in samples containing Er^{3+} and $\text{Er}^{3+}/\text{Yb}^{3+}$. In Er^{3+} doped glasses, green and red emissions are recorded together with a dominant band near 1530 nm, accompanied by weaker NIR transitions. When co doped with Yb^{3+} , a substantial enhancement of both downshifting and up conversion luminescence is obtained due to $\text{Yb}^{3+} \rightarrow \text{Er}^{3+}$ energy transfer, including the appearance of an intense emission near 900 nm under 980 nm excitation. In Ho^{3+} doped samples, the expected green and near infrared emissions associated with Ho^{3+} multiplet transitions are identified. Across all RE doped compositions, photoluminescence intensities are found to vary systematically with dopant concentration. Lifetime measurements of the relevant excited states are included alongside the spectral data to provide complementary insight into radiative and non radiative relaxation pathways. Overall, the results indicate that RE doped $\text{PbCl}_2\text{-BiO}_3/2\text{-TeO}_2$ glasses form a versatile platform for visible and near infrared photonic applications, offering strong downshifting emission and tunable up conversion responses suitable for sensing and related optical technologies.

One-dimensional crystalline polymer regulated by non-covalent interactions

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Tuning the dimensions and molecular packing geometry of crystalline organic frameworks and polymers represents an important challenge for reticular chemistry. At the same time, installing different chemical entities onto crystalline frameworks with well-defined spatial distributions represents a viable approach to achieving ordered and complex synthetic materials. Here, we first show a covalent organic framework (COF-305) is constructed from tetrakis(4-aminophenyl)methane and 2,3-dimethoxyterephthalaldehyde, which has the largest unit cell and asymmetric unit among known COFs. The insight provided by COF-305 supplements the principle of covalent reticular design from the perspective of non-covalent interactions and opens opportunities for pursuing complex chemical sequences in molecular framework. Then we show that for extended structures made of 1,3,6,8-tetrakis(4-aminophenyl)pyrene (PyTTA) linked with methoxy group functionalized terephthalaldehyde aldehydes, simple substituents on the aldehyde linker can have profound structure directing effects due to noncovalent interactions. Specifically, reacting 2,3-dimethoxyterephthalaldehyde with PyTTA gives a 2D covalent organic framework with unique AA-inclined-AA stacking and bilayer pyrene motifs, whereas reacting 2,5-dimethoxyterephthalaldehyde with PyTTA gives a 1D crystalline polymer with AB stacking and isolated pyrene motifs. Both materials show high crystallinity, allowing for atomic resolution structure determination using three-dimensional electron diffraction, and the similarity of their fluorescence properties shows the electronic structures of pyrene-based extended structures mostly depends on the in-plane structures, which is supported by density functional theory calculations. These two pyrene-based extended structures also show different fluorescence responses to organic vapors due to different pore environments. The current work shows the potential of noncovalent interactions in the reticular design of functional organic materials. It also leads us to the synthesis of one-dimensional crystalline

polymers regulated by non-covalent interaction. It exhibits attractive characteristics in various aspects such as tunability, proton conductivity, and porosity.

Reticulating Node-Linker-Modulator Chemical Space for Alkoxide-Based Molecular Network-Forming Glass

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Molecular network-forming glasses are emerging type of hybrid glasses subjected to intensive research in recent years. In this work, we investigate alkoxide-based glasses and liquids composed of metal nodes (Ti, Zr, B), multidentate alcohol linkers, and monodentate alcohol modulators within a node–linker–modulator framework. This design allows precise control over coordination environments and intermolecular interactions, enabling systematic investigation of structure–property relationships across a wide compositional range. By tuning the composition, we examine the evolution of structure and dynamics using rheological, thermal, and structural characterization techniques, providing insight into how molecular-scale interactions translate into macroscopic properties. Results show that decreasing the modulator content promotes network connectivity, which is reflected by a pronounced increase in viscosity and the emergence of glassy behavior. At higher modulator concentrations, the system is dominated by discrete or weakly interacting species, leading to liquid-like behavior with relatively low viscosity and high molecular mobility, whereas reducing the modulator fraction facilitates the formation of extended coordinative networks, restricting molecular motion and promoting glass formation. This compositional control enables a continuous transition from molecular liquids to extended network structures over a broad compositional window, accompanied by significant changes in viscoelastic response. Furthermore, the glass transition temperature is governed by the balance between network connectivity and intermolecular interactions, reflecting the combined effects of coordination bonding and secondary interactions.

Synthesis of Niobium Alkoxide Based Network-Forming Glass

Yidan Song, ShanghaiTech University

Niobium alkoxide clusters possess abundant coordination sites and are thus suitable for constructing inorganic-organic hybrid glass networks via ligand exchange reactions with polyols or phenolic ligands. In this work, we utilize niobium ethoxide as a precursor alongside flexible-chain alcohols and rigid phenols as organic building units to investigate the influence of ligand structure on glass formation and network tunability. For the flexible alcohol system, small-molecule modulators are introduced to regulate the transesterification and equilibrium processes between the niobium centers and hydroxyl groups during solvent evaporation. This regulation achieves dynamic and reversible control over the glass structure, flowability, and processability. Conversely, in the rigid phenol system, the stronger driving force for coordination and condensation favors the formation of more rigid networks. However, introducing small-molecule modulators effectively reduces the local crosslinking degree and delays network solidification, which allows for dynamic and reversible transitions between different glass states. This study provides new strategies for designing metal alkoxide-based hybrid glasses and offers a theoretical foundation for developing novel glass materials with enhanced processability, self-healing capabilities, and repeatable formability.

Integrated multi-mode optical thermometry in Mn²⁺, Tm³⁺, and Yb³⁺ co-doped oxyfluoride glass and glass-ceramics containing KZnF₃ nanocrystals

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Temperature measurement is often limited by the slow response and sample disturbance inherent to contact sensors, especially at small scales. Opposite, optical thermometry offers a fast, non-contact alternative with high temperature and spatial resolution, suitable for harsh environments. Among the various optical parameters used to measure the temperature, the

fluorescence intensity ratio (FIR) is particularly reliable. This is because it is largely immune to external disturbances and does not require calibration, making it highly promising for accurate temperature sensing in challenging conditions. In this work, we propose a new class of Mn-activated oxyfluoride glasses (OxG) and glass-ceramics (OxGC) containing KZnF_3 nanocrystals for optical thermometry applications. Oxyfluoride systems offer low phonon energy, enabling efficient incorporation of luminescent ions, while KZnF_3 provides a highly suitable crystalline host for transition-metal and rare-earth ions. Although Mn^{2+} -doped KZnF_3 nanocrystals have demonstrated tunable broadband red emission through crystal-field-dependent d–d transitions and Mn–RE energy transfer, no studies to date have investigated their potential for temperature sensing. To address this gap, this study aims to optimize Mn^{2+} incorporation in the KZnF_3 phase and explore co-doping with Tm^{3+} , and Yb^{3+} to achieve dual-emission behavior suitable for optical FIR thermometry. Mn-based broadband emission, combined with the sharp f–f transitions of Tm^{3+} and Yb^{3+} , offers two thermally responsive channels for FIR-based calibration. Building on previous results where Er^{3+} - and Tm^{3+} -doped OxGCs exhibited strong upconversion and reliable temperature dependence, the Mn/Tm, and Mn/Tm/Yb systems will be examined under NIR excitation to establish temperature sensitivity and thermometric precision. This work introduces the first Mn-activated KZnF_3 -based glass-ceramic platform for optical thermometry, providing a promising route toward robust, broadband, and dual-emission temperature sensors for advanced photonic and industrial applications.