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Modelling Monolayer MoS_2 in an External Electric Field with Tight Binding

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1. Introduction

Usage of 2D materials in modern devices has been a field of great interest in recent years. 2D materials can be made atomically thin, making them great for nano-sized devices, and they often possess unique or noteworthy physical properties. MoS_2 is a 2D material of particular interest as it is a semiconducting 2D material, making it a great candidate for usage in electrical and optical devices.

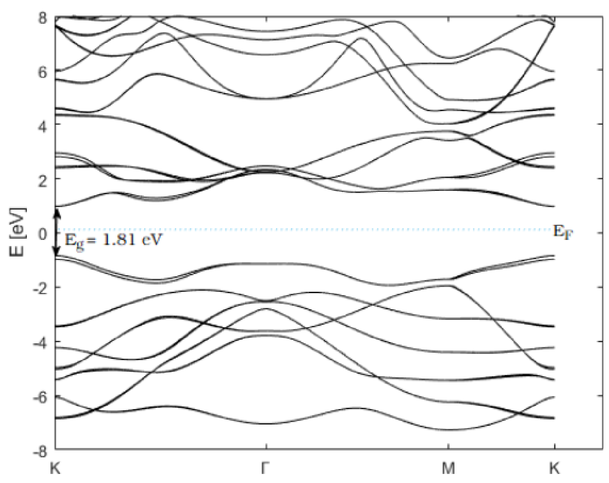
The electrical and optical properties of materials are primarily determined by which energy states its electrons can occupy, as described by their band structure. This therefore makes it interesting to be able to change and tune the band structure of a MoS_2 monolayer especially its bandgap. A model was constructed to investigate how the band structure of MoS_2 would react and change in an electric field.

2. MoS_2 band structure

A tight binding model was utilized in order to calculate the band structure. This model takes into account the interactions of the various electrons orbitals within a structure through the equation

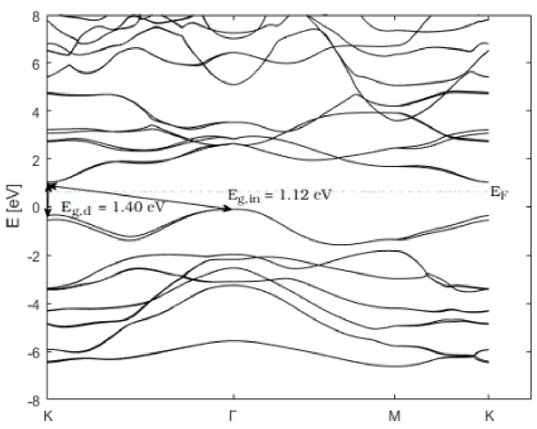
$$\bar{\mathbf{H}} \cdot \mathbf{c} = E\bar{\mathbf{S}} \cdot \mathbf{c}$$

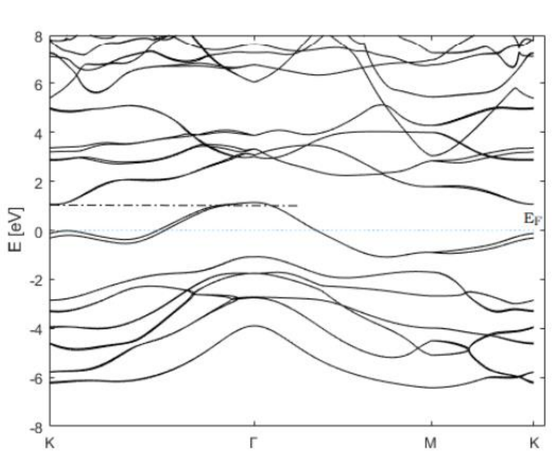
Where H is the interaction energy, S is the overlap between orbitals, c is an eigenvector, and E is the band energy. The band energy can be evaluated by calculating the H- and S-matrices.



It can be seen that the band structure of MoS_2 with no electric field applied has a direct bandgap of 1.81 eV in the K point. The presence of a direct bandgap is critical for the performance of many opto-electronic devices.

The lower bands shift upwards as an external electric field is applied, with the bands changing particularly rapidly in the Γ point. This causes the bandgap to become indirect, and eventually disappear, turning the material metallic.

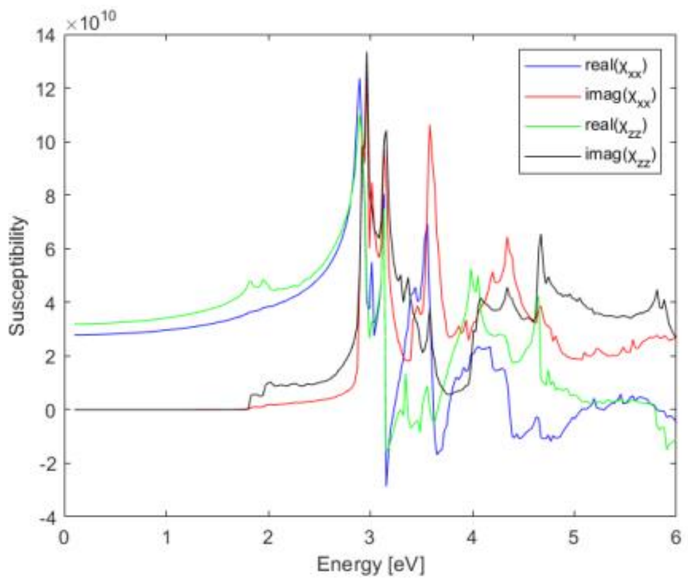


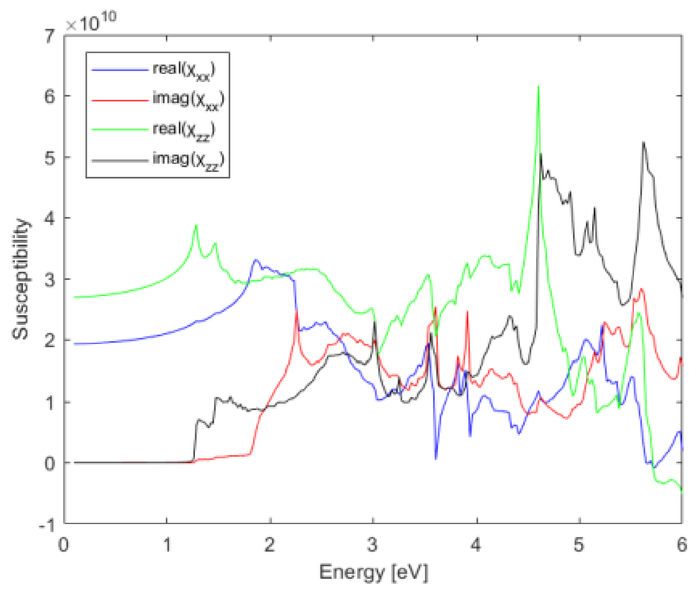


3. Susceptibility

The band structure was utilized in order to calculate susceptibility and conductivity of the MoS_2 monolayer.

The susceptibility has both a real and imaginary part, where the real part describes how the material reacts to an electric field, while the imaginary part is proportional to the material's absorbance.
With no applied electric field the material does not start absorbing light until the energy of the incoming photons are equal to the bandgap at 1.8 eV.





As the electric field is applied and the bandgap narrows, it can be seen that the structure also starts absorbing light at lower photon energies. Photons can only cause direct transitions between the bands, so the photons still need a certain energy before they can be absorbed, even in the metallic case.

4. Conclusions

A mathematical model was constructed in order to calculate the band structure of a MoS_2 monolayer. This model was utilized in order to investigate how the band structure was modified by an external electric field. The electric field had an especially pronounced effect on the bands around the Γ point, which caused the band structure to change from direct to indirect and then metallic with increasing electric field strength.

It could also be seen that the changing band structure had an effect on the electric properties of MoS_2 monolayers. The susceptibility and conductivity were generally decreased as a stronger field was applied, weakening its response to other external electric fields.

Acknowledgement

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