Modelling Monolayer MoS₂ in an External Electric Field with Tight Binding

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Abstract

This project modelled the band structure of a monolayer of the transitional-metal dichalcogenide molybdenum disulfide (MoS₂) through the use of the tight binding method. While the properties of MoS₂ have been of major scientific interest for many years, this project investigated an aspect of the 2D material which is not well researched. Namely, how a vertical external electric field affects the band structure, and certain electrical and optical properties of a MoS₂ monolayer. MoS₂ monolayers are known to have a direct bandgap of ≈ 1.8 eV. By applying an external electric field of $\varepsilon = 5.52$ V/Å, the bandgap both decreased to 1.12 eV and was found to shift from direct to indirect. Furthermore, increase in external electric field strength to $\varepsilon = 10.9$ V/Å caused the bandgap to disappear entirely. Finally, external electric fields were also found to generally decrease the susceptibility and conductivity of MoS₂ monolayers as the electric field strength increased.

Keywords: Tight Binding, MoS2, Monolayer, Electric Field

1. Introduction

There has been considerable interest in research into MoS_2 . Being a semiconductor material, it has a notable potential in regards to electronics and photonics [1]. Especially microelectronics have been of interest for research into MoS_2 . Bulk MoS_2 has an indirect bandgap of 1.2 eV, but single layers of MoS_2 instead act as direct bandgap semiconductors with a bandgap of 1.8 eV. This has garnered interest into their usefulness as switchable transistors and as photodetectors [2, 3]. Additionally, MoS_2 has been shown to demonstrate superconductivity [4]. Finally, MoS_2 has also been identified as an efficient catalyst for hydrogen gas for fuel cells [5]. An important tool in moving towards a more sustainable power supply.

 MoS_2 is a layered transition metal dichalcogenide. Each layer is only connected to the other layers by weak van der Waals forces, and it is therefore possible to obtain a thickness of a single layer [6]. This is a useful property in regards to creating nanoscale devices, as many of the aforementioned research is working on such devices. A significant portion of this research has been aimed at examining the feasibility of modifying the bandgap of MoS_2 for use in nanoscale electronic devices [7, 8, 9], where especially the utilization of strain as a method to modify the bandgap properties has been attempted [10, 11].

This project will model and investigate the MoS_2 structure on an atomic basis through the use of the TB model. This will grant a better understanding of the band structure and behaviour of the 2D material. The model will be used to investigate the effect of an external electric field on the properties of the bandgap of a MoS_2 monolayer. As well as how an external electric field affects the electrical properties of susceptibility and conductivity.

2. Tight Binding Method

In order to model the electronic properties of 2D materials, the TB method, sometimes called LCAO, is utilized. The relevant theory for this model will be presented here.

The TB model arises from the field of quantum mechanics. As with many parts of quantum mechanics, the fundamental equation for the foundation of the TB model is the time-independent Schrödinger equation

$$\hat{H}|\Psi\rangle = E|\Psi\rangle,\tag{1}$$

where \hat{H} is the Hamilton operator (also called the Hamiltonian), Ψ is the wavefunction, and *E* is the

energy of the system. This equation is an eigenvalue equation. To model the 2D materials of interest to this project, it is necessary to solve this equation for a oneelectron Schrödinger equation in a special set of basis functions. The basis are the atomic orbitals of interest to the system, and depend greatly on the constituent atoms of the system and their orientation in relation to each other. In the case of a single particle the Schrödinger equation is of the form

$$\hat{H}|\psi\rangle = (T+V)|\psi\rangle = E|\psi\rangle,$$
 (2)

where *T* is the one-electron kinetic energy, and V is the effective potential in a mean-field approximation. The basis functions of the wavefunction are commonly written on the form $|\mathbf{n}, i, \mu\rangle$. Here, **n** denotes the lattice vector \mathbf{R}_n , *i* denotes the *i*-th basis atom, and μ denotes the type of orbital.

It is now assumed that the solution can be written in the form of a linear combination of atomic orbitals, and if so it is possible to take the sum

$$|\psi\rangle = \sum_{\mathbf{n},i,\mu} c_{\mathbf{n},i,\mu} |\mathbf{n},i,\mu\rangle, \qquad (3)$$

where $|\psi\rangle$ now represents the molecular orbital created by the sum of atomic orbitals ($|\mathbf{n}, i, \mu\rangle$), and $c_{\mathbf{n},i,\mu}$ is a coefficient which is multiplied with each atomic orbital. By inserting 3 into 2 one gets.

$$\sum_{\mathbf{n},i,\mu} c_{\mathbf{n},i,\mu} \hat{H} |\mathbf{n},i,\mu\rangle = E \sum_{\mathbf{n},i,\mu} c_{\mathbf{n},i,\mu} |\mathbf{n},i,\mu\rangle.$$
(4)

Applying $\langle \mathbf{m}, j, \nu |$ the expression becomes

$$\sum_{\mathbf{n},i,\mu} c_{\mathbf{n},i,\mu} \langle \mathbf{m}, j, \nu | \hat{H} | \mathbf{n}, i, \mu \rangle = E \sum_{\mathbf{n},i,\mu} c_{\mathbf{n},i,\mu} \langle \mathbf{m}, j, \nu | \mathbf{n}, i, \mu \rangle,$$
(5)

where \mathbf{m}, j, ν likewise denotes a lattice vector, the *j*-th atom, and the type of orbital, respectively. This equation can be constructed for the other orbitals as well.

This equation can be converted into a matrix equation instead. This results in a generalized matrix eigenvalue problem, succinctly written as

$$\bar{\mathbf{H}} \cdot \mathbf{c} = E\bar{\mathbf{S}} \cdot \mathbf{c},\tag{6}$$

where **c** is the coefficient vector for the linear combination of the eigenstate $|\psi\rangle$, similar to the role in the 'standard' equation, and $\overline{\mathbf{H}}$ and $\overline{\mathbf{S}}$ are the Hamiltonian and overlap matrices, respectively. $\overline{\mathbf{H}}$ and $\overline{\mathbf{S}}$ are represented in the basis of the atomic orbitals and correspond to entries as seen below

$$H_{ni\mu}^{mj\nu} = \langle \mathbf{m}, j, \nu | \hat{H} | \mathbf{n}, i, \mu \rangle \tag{7}$$

$$S_{ni\mu}^{mj\nu} = \langle \mathbf{m}, j, \nu | \mathbf{n}, i, \mu \rangle.$$
(8)

2.1 Parametrization of the Hamiltonian and Overlap Matrices

The matrix terms $H_{0i\mu}^{nj\nu}$ and $S_{0i\mu}^{nj\nu}$ are determined by studying the terms which appear in the integral. The Hamiltonian matrix is studied, and to simplify things a one-atom basis is considered. This can be seen below

$$H_{0\mu}^{0\nu} = \int \phi_{\mu}^{*}(\mathbf{r})(T+V)\phi_{\nu}(\mathbf{r}-\mathbf{R}_{n})d\mathbf{r}$$
$$= \int \phi_{\mu}^{*}(\mathbf{r})(T+(\sum_{m} v_{at}(\mathbf{r}-\mathbf{R}_{m})))\phi_{\nu}(\mathbf{r}-\mathbf{R}_{n})d\mathbf{r},$$
(9)

where ϕ_{μ} is the wave function of orbit μ , and $v_{at}(\mathbf{r} - \mathbf{R}_m)$ is the atomic potential of the atom in the *m*'th unit cell. This leads to a few different types of integrals for the potential energy. Namely the one-, two- and three-center integral. The last of these is neglected, as they are generally fairly small for atomic orbitals. However, the first two are relevant, and will be presented here.

The one-center integral can be expressed as

$$\int \phi_{\mu}^{*}(\mathbf{r}) v_{at}(\mathbf{r}) \phi_{\nu}(\mathbf{r}) d\mathbf{r}.$$
 (10)

For these integrals there are two scenarios of interest. Either $\mu = \nu$ or $\mu \neq \nu$. If $\mu = \nu$ then the integral corresponds to the typical on-site energy (ϵ_{μ}) for the μ atomic orbital. If $\mu \neq \nu$ then its contribution is small assuming $\langle \phi_{\mu} | \phi_{\nu} \rangle \neq 0$ The two-center integral can be split into two forms (here called '1' and '2'). Two-center integral 1 can be expressed as

$$\int \phi_{\mu}^{*}(\mathbf{r}) \sum_{n \neq 0} v_{at}(\mathbf{r} - \mathbf{R}_{m})) \phi_{\nu}(\mathbf{r}) d\mathbf{r}.$$
 (11)

If $\mu = \nu$, then the integral contributes to the on-site energy, as a result of the other atoms. If $\mu \neq \nu$, then the contribution is termed a 'hopping element', and is also a result of the other atoms.

Two-center integral 2 can be expressed as

$$\int \phi_{\mu}^{*}(\mathbf{r}) v_{at}(\mathbf{r})) \phi_{\nu}(\mathbf{r} - \mathbf{R}) d\mathbf{r}, \mathbf{R} \neq 0.$$
(12)

These integrals also contribute the hopping elements, which describes the electron transition between two different orbits. As a final important note, the matrix elements which describe the kinetic energy T are unchanged for both one-center and two-center integrals. This means they also contribute to the on-site and hopping energies [12].

Unfortunately, determining these integrals can be rather complicated. The next section will introduce a method to simplify the process.

2.2 Slater-Koster Method

The method introduced by Slater and Koster [13] is an interpolation method. It simplifies the determination of the integrals by instead reducing them to constants at the points of symmetry within the BZ, thereafter allowing them to be used for calculations throughout the whole BZ. This means the TB model is much simpler, as it can be solved by only considering some parameters.

The method works by considering the interaction of the orbitals. More specifically, it uses the angular dependence of the $(\phi_{\nu}(\mathbf{r} - \mathbf{R}))$, which is described by the s-, p-, and d-orbitals, to determine the angular dependence of hopping energies for each type of orbital interaction. The orbitals are linear combinations of the spherical harmonics, and as such, the hopping elements consist of the following matrix elements of \hat{H} with the spherical harmonic functions $|l, m\rangle$

$$V_{ll'm}^{i \to j} = \langle \mathbf{n}, i, l, m | \hat{H} | \mathbf{n}', j, l', m' \rangle.$$
(13)

Here l,l' represent the angular-momentum quantum number of the orbitals, and m, m' represent the magnetic quantum number. The magnetic quantum numbers m and m' must be the same because of selection rules.

The hopping elements of the Hamiltonian of s-, p-, and d-orbitals can be expressed as a linear combination of the ten types of Slater-Koster parameters (had the three-center integral been included, more parameters would have been necessary). The ten relevant linear combinations can be seen in figure 1.

Each linear combination will consist of two of these orbital types, and will express a type of bonding symmetry. The relevant symmetries are commonly labeled σ, π or δ .



Fig. 1 The ten linear combinations of the possible s-, p-, and d-orbitals, which represent the ten Slater-Koster parameters. The red and yellow colors indicate the polarization (+ or -) of the orbitals [14].

Each of these ten Slater-Koster parameters are linear combinations of the matrix elements as presented in equation 13. Returning to this equation it is possible to introduce some simpler notation. The l,l' and m in the $V_{ll'm}$ notation can instead more directly show the orbital interaction in question. The l and l' can be replaced by the type of orbital (s-, p-, or d-type), previously denoted μ and ν , since this is what the angular momentum describes. Likewise the *m* stands for one of the three bonding symmetries. As an example, interaction between and s-orbital and a p-orbital can

therefore be given the notation $V_{sp\sigma}$.

The ten Slater-Koster parameters are sufficient to describe a system which consists of one atom per unit cell (so i = j), but importantly where only nearest-neighbor interaction along the z-axis is considered. Applying the notation to all possible ten Slater-Koster parameters, as seen in figure 1, with those considerations in mind, and inserting them into the Hamiltonian matrix yields a 9x9 matrix.

If $i \neq j$, then these values must be determined separately. The values within the matrix therefore depend greatly on the exact atoms in the lattice and their crystal structure/orientation. The parameters must therefore be determined for each pair of atoms in the basis being modelled, since the Hamiltonian also depends on the distance between atoms.

Since there is an angular dependence of the spherical harmonic functions, all of the hopping energy elements along a random orbital bonding direction **R** can be expressed by these linear combination of the ten Slater-Koster parameters. This means it is possible to take the matrix seen in equation ?? (which is for hopping energy elements for a bonding direction along the z-axis), and rotate it into the corresponding matrix with hopping energy elements along the **R**-direction. Doing this is called a Slater-Koster transformation.

A simple example of a hopping element between two orbitals can be seen in figure 2.



Fig. 2 Slater-Koster transformation for a s-orbital and a p_z -orbital. The left-most orbital combination $(H_s^{p_z})$ is a linear combination of the other two cases $(V_{sp\sigma} \text{ and } V_{sp\pi} \text{ from left to right)}$ [12].

The notation on figure 2 can be further simplified by utilizing the unit vector of **R**. Then, the unit vector's components, $\bar{\mathbf{r}} = \frac{\mathbf{R}}{|\mathbf{R}|} = (l \ m \ n)^T$, can be utilized rather than cos and sin functions. This would change the equation shown on 2 into

$$H_s^{p_z}(\mathbf{R}) = n \cdot V_{sp\sigma},\tag{14}$$

which is the method of implementation used in this project [12].

Once the matrix elements of all orbitals have been calculated, the energies of electrons at all points within the first BZ are known. This can be summarized in a band structure graph.

To get a fully correct band structure, the spin orbit coupling (SOC), must also be taken into account. This will not be elaborated here, however, a derivation of it can be found in chapter 10 of [15].

2.3 External Electric Field

To model the effect of an external electric field on the MoS₂ monolayer, the necessary components for describing a static (\hat{H}_0) electric field will be determined.

The energy of a charged particle in a static electric field is

$$E = \vec{\varepsilon} q \vec{r}.$$
 (15)

If the electric field is parallel with the z-axis, then eq. 15 becomes

$$E = \varepsilon q z, \tag{16}$$

where q is the electric charge. This makes the Hamiltonian for the system

$$\hat{H}_0 = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right) + \varepsilon qz. \tag{17}$$

The terms within the parenthesis are the energy contributions from the momentum of the electron and the potential field of the nucleus. These energy contributions are accounted for within the tight-binding model. As such, the energy contribution from the external electric field may simply be added on top of the energy calculated through the tight-binding model

$$\langle \varphi_n | \hat{H}_0 | \varphi_m \rangle = E_{nm} + \varepsilon q \langle \varphi_n | z | \varphi_m \rangle.$$
 (18)

The function $\langle \varphi_m | z | \varphi_n \rangle$ can be simplified further by choosing a reference point which lies between the two atoms under consideration

$$\langle \varphi_n | z | \varphi_m \rangle = \langle \varphi_n | z - \bar{z} | \varphi_m \rangle + \bar{z} \langle \varphi_n | \varphi_m \rangle, \quad (19)$$

where \bar{z} is the average z-value for the two orbitals. The first term in eq. 19 disappears, since z is an even function and φ is an odd function. The second term, $\langle \varphi_n | \varphi_m \rangle$ is simply the overlap between the atomic orbitals. This then gives the final equation

$$\Delta H = \varepsilon q \bar{z} S_{nm}.$$
 (20)

As the derivation of the equation for the implementation of the electric field is done with the electric field parallel to the z-axis, this is the direction it will be implemented in the code. This means that any mention of the electric field in later sections refer to an electric field perpendicular to the MoS₂ monolayer.

With this theory in mind, a MatLab program was produced to model the band structure in the presence of a static external electric field.

3. Band Structure in Electric Fields

A plot of the band structure without any applied external fields can be seen on figure 3.



Fig. 3 Modelled band structure when considering the s-, p-, and d- orbitals in MoS_2 with SOC taken into account. The dotted line marks the Fermi level of $E_F = 0.121$ eV, and the double arrow indicates the bandgap energy of $E_g = 1.81$ eV.

As can be seen on figure 3, the band structure has a direct transition in the K point equal to $E_g = 1.81$ eV.

Having constructed a TB model of the band structure of MoS_2 , it is of interest to investigate how this band structure changes in response to the presence of a vertical static external electric field. Figure 4 shows the band structure of MoS_2 in an electric field strength of 7.2 V/Å.



Fig. 4 Modelled band structure of MoS₂ with SOC taken into account. An electric field of strength $\varepsilon = 7.2$ V/Å has been applied across the width of the monolayer. The dotted line marks the Fermi level of $E_F = 0.121$ eV, and the double arrow indicates the bandgap energy of $E_g = 1.81$ eV.

At this external electric field strength, and interesting development has occurred. Namely the bandgap has shifted from being a direct bandgap in K to an indirect bandgap from the Γ point in the valence band (VB) to the K point in the conduction band (CB). The shift already occurred at an external electric field strength of 5.52 V/Å.

In general, as the strength of the electric field increases, all bands increase slightly in energy. The order of the bands does not change relative to each other, but their exact shape and curvature does. The bands which were split as a result of taking SOC into account are further split while in an electric field. However, the electric field has not changed the regions in which the split is observable.

The results found here agree with the findings of the couple of other similar articles. The two articles modelled a flat MoS₂ monolayer with an applied a perpendicular electric field through DFT calculations. C. V. Nguyen et al. (2016) [16] determined that applying a perpendicular electric field strength of 0.6 V/Å across a MoS₂ monolayer causes the bandgap to decrease and shift from direct to indirect. In agreement with the findings of this project, they determine a direct bandgap from K in the VB to K in the CB, which switches to an indirect from Γ in the VB to K in the CB. Zibouche et al. (2014) [17] observed the same switch from direct to indirect at these points. While it is not specified precisely at which external electric field strength they observed this switch, it is shown to only barely have happened at electric field strength of 3 V/Å, which is comparable to the 5.52 V/Å found in this project.

While all bands increase slightly in energy, as strength of the external electric field is increased, some regions of k-space increase faster than others. This is especially true in the Γ point in the VB. The greater increase in the energy of the VB in the Γ point has the interesting consequence that by increasing the strength of the electric field enough, the MoS₂ monolayer modelled changes from being a semiconductor material to a conductor material instead. This shift occurs at field strength of approximately 10.9 V/Å, at which point the energy of the VB in the Γ point is virtually identical with that of the energy of the CB in the K point. This phenomena is observable in figure 5.



Fig. 5 Modelled band structure with SOC in the presence of an electric field at a strength of 11 V/Å. Important to note is the energy of the VB at Γ is higher than that of the CB at K, meaning the band structure no longer exhibits semiconductor band structure. The dashed and dotted line highlights the energy of the CB at the K point. $E_F = 0.007$ eV.

This effect has major implications for the use of MoS_2 monolayers in nanoelectronics and optical devices, since it allows for construction of a tunable bandgap. Allowing for switching between semiconductor and conductor material properties. Although the electron would need to change its momentum, since the bandgaps do not meet directly in k-space, but simply have comparable energies. This could for instance be accomplished by a scattering process.

4. Electrical Properties

Returning to the band structure with SOC and no external electric field, this band structure was used to investigate the electrical properties of MoS2. The exact electrical properties investigated are the susceptibility (χ) and conductivity (σ) , while investigating either the absorption can be partially identified, since particular properties are proportional to it. After calculating them with no external field, the same properties were determined under various electric field strengths. The energies modelled on the x-axis on graphs in this section should be imagined as energy provided by photons with energy $E = \hbar\omega$.

4.1 Susceptibility

The real (Re) and imaginary (Im) parts of χ_{xx} and χ_{zz} for a MoS₂ monolayer as modelled in this project with no external field can be seen in figure 6



Fig. 6 Susceptibilities of the modelled MoS₂ monolayer with no external electric field. The blue, red, green and black lines correspond to $\text{Re}\chi_{xx}$, $\text{Im}\chi_{xx}$, $\text{Re}\chi_{zz}$, and $\text{Im}\chi_{zz}$, respectively. x-axis: Energy in [eV], y-axis: Susceptibility, χ

 $\chi_{xx} = \chi_{yy}$, which is why only one of them has been plotted. The Re parts are the susceptibility itself, while the Im parts are proportional to the absorption.



Fig. 7 Susceptibilities of the modelled MoS₂ monolayer with an external electric field of 11 V/Å. The blue, red, green and black lines correspond to Re χ_{xx} , Im χ_{xx} , Re χ_{zz} , and Im χ_{zz} , respectively. x-axis: Energy in [eV], y-axis: Susceptibility, χ

In all cases, the Im parts start at zero, while the Re parts start above zero. The Re parts starting above zero indicates that a MoS₂ monolayer always possesses an inherent susceptibility. Likewise the Im parts starting at zero indicates that absorption does not take place until sufficient energy is present in the photon such that electronic excitations are possible. Increases to Re parts can be interpreted as an increase in available transition states, while peaks in Im parts are expected to appear at energies which equal the energy between the VB and CB bands. The Re and Im plots of both χ_{xx} and χ_{zz} follow each other closely, with peaks and dips at the same energies, this is a result of certain energy levels having an abundance of transitions between different bands, increasing both the ease by which electrons can get excited, and the number of available states.

The case of no external electric field is considered first. Starting from 0 eV the Re parts initially both increase gradually with increasing energy, while the Im parts are unchanged. At around 1.8 eV all plots increase in susceptibility, which is expected, since this is energy corresponds to the bandgap. Re χ_{zz} and Im χ_{zz} exhibit two clear peaks here, which are a result of the split VB due to SOC, this is supported by the distance between the dual peaks being ≈ 0.14 eV, which corresponds to the splitting in K.

As the energy increases further, there is a slow but steady rise in susceptibility until about 2.7 eV, where all plots increase sharply. Looking at fig. 3, it can be seen that there is an interval roughly halfway between K and Γ where the curvature of the VB and CB are similar. This region creates a large number of possible transition states, and since the energy differential between the CB and VB is approximately 2.8 eV, it corresponds well with the observed increase in susceptibility.

Further increasing the energy to approximately 3.5 eV results in another spike in the $\text{Re}\chi_{xx}$ and $\text{Im}\chi_{xx}$ plots, which could be explained by considering the bandgap at and around the Γ point, where the relatively flat VB and CB allow for many possible electronic excitations, since there are a large number of available states in the CB, as many bands overlap in this region. Generally, the differences in χ_{xx} and χ_{zz} highlight the anisotropic nature of the MoS2 monolayer.

Moving on to the susceptibilities with various external electric field strengths, it is interesting to compare with no external field, and consider the differences.

In general, the starting values of the Re plots decrease as the strength of the external electric field is increased. Both starting at a susceptibility of around 2.8 and 3.2 with an external electric field strength of 0 V/Å, and ending at around 1.9 and 2.8 with an electric field strength of 11 V/Å for χ_{xx} and χ_{zz} , respectively. Meaning χ_{xx} is significantly more susceptible to the effects of an external electric field. The Im plots still remain at zero susceptibility until the bandgap energy is reached.

Following the twin peaks in Re and Im χ_{zz} , which represent the bandgap and were discussed earlier, it is clear that as the strength of the external electric field increases, they are redshifted as the bandgap decreases in energy. Interestingly, while the twin peaks are initially quite comparable in susceptibility, as the strength of the electric field increases, the one peak increases more rapidly, and is noticeably higher with an external electric field strength of 11 V/Å. It is the first peak that exhibits this behaviour, or in other words, the split VB at the K point with the highest energy. At the same time, the distance between the peaks has increased slightly. This coincides well with the increased distance between the VB at K in figure 5.

4.2 Conductivity

The real and imaginary parts of σ_{xx} and σ_{zz} for a MoS2 monolayer as modelled in this project with no external field, can be seen in figure 8. As described previously, $\sigma_{xx} = \sigma_{yy}$, which is why only σ_{xx} is shown. The Re parts constitute the conductivity in the physical sense of the ability of an electric field to move an electron. The discussion of the conductivity will focus on the Re parts.

Starting from 0 eV, the conductivity remains at zero until the energy of the bandgap (1.8 eV) is reached. Again, the split VB as a result of SOC is visible as two small increases in $\text{Re}\sigma_{zz}$. From this point on, the conductivity increases slowly until about 2.7 eV, at which point there are two consecutive massive peaks in conductivity. As with susceptibility, these peaks can be explained by these energies constituting direct bandgap energies between K and Γ , and around Γ , respectively. Since an electron excited into the CB is able to move around more freely in a semiconductor material, thus increasing the conductivity at these energies.

It can be seen that as the strength of the E-field increases, the real part of σ_{xx} gradually flattens out. This flattening primarily effects the peaks before 4 eV, while the general shape and magnitude of the conductivity after 4 eV was preserved. This same effect was also observed for the susceptibility, and there are two potential causes for this. The first relates to the fact that magnitude of the conductivity and susceptibility



Fig. 8 Conductivities of the modelled MoS₂ monolayer with no external electric field. The blue, red, green and black lines correspond to $\text{Re}\sigma_{xx}$, $\text{Im}\sigma_{xx}$, $\text{Re}\sigma_{zz}$, and $\text{Im}\sigma_{zz}$, respectively. x-axis: Energy in [eV], y-axis: Conductivity, χ



Fig. 9 Conductivities of the modelled MoS₂ monolayer with an external electric field strength of 7.2 V/Å. The blue, red, green and black lines correspond to $\text{Re}\sigma_{xx}$, $\text{Im}\sigma_{xx}$, $\text{Re}\sigma_{zz}$, and $\text{Im}\sigma_{zz}$, respectively. x-axis: Energy in [eV], yaxis: Conductivity, χ

are both related to the number available states, and the electric field causes the bands to spread out evenly, resulting in fewer peaks of the transition states. The other hypothesis is that both the susceptibility and conductivity both relate to how the material responds to an external electric field. However, since the strong electric field which has been applied to the material may have saturated it, weakening its response to any further fields.

5. Conclusion

The project succeeded in constructing a mathematical model of the band structure of a MoS₂ monolayer. This model was then expanded to include the effects of SOC, which caused some bands within the band structure to split in energy in regions around the K point, while the only effect on other regions was the splitting of degenerate bands at the Γ point.

The model with SOC predicts a direct bandgap of $E_g = 1.81$ eV at the K point in good agreement with models from previous studies.

The model was then further expanded to model the effect of a static electric field on the band structure. In general, increasing the strength of the electric field increased the energies of the bands. Especially energies in the Γ point where susceptible to the effects of an applied electric field. An applied electric field strength of $\varepsilon = 5.52$ V/Å caused the MoS₂ monolayer to shift

from a direct bandgap at K to an indirect from Γ in the VB to K in the CB. Further increase in the electric field strength to $\varepsilon = 10.9$ V/Å caused the bandgap to disappear entirely, presenting an intriguing use of applying a vertical electric field as a means of tuning the bandgap of a MoS₂ monolayer. Thus changing the material properties from semiconductor to conductor.

Finally, the model was expanded to model the susceptibility and conductivity of a MoS₂ monolayer with and without an external electric field, in order to determine how the presence of an external electric field affects these electrical properties. In general, both susceptibility and conductivity were found to decrease as the strength of the electric field increased.

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