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Electronic and Dielectric Properties of MoS$_2$-MoX$_2$ Heterostructures

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Abstract. We present a comparative study of electronic and dielectric properties of MoS$_2$-MoX$_2$ heterostructures (where X=S, Se, Te) within the framework of density functional theory (DFT). Electronic band structure, real & imaginary part of dielectric function, electron energy loss spectra and static dielectric constant have been calculated for each system and compared with one another. A systematic decrease/increase in band gap/static dielectric constant is observed as the X changes from S to Te. These results provide a physical basis for the potential applications of these heterostructures in optoelectronic devices.

Keywords: DFT, Electronic properties, Dielectric properties.

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INTRODUCTION

Two dimensional (2D) layered transition metal dichalcogenides (TMDs) have attracted a great deal of interest [1-4] due to their capabilities to fulfil the demands of nano-electronics industry. The direct band gap in TMDs monolayers [3] make them a suitable material for optoelectronic devices. In the recent time efforts have been devoted to control the direct band gap character in multilayers by means of heterostructuring [5,6]. Very recently, the successful experimental synthesis of TMDs heterostructures have been reported [7]. In the present study, our aim is to explore and compare the changes in electronic and dielectric properties of MoS$_2$-MoX$_2$ heterostructures (where X =S, Se, Te) with the change in chalcogen atom in one layer with respect to other layer. For this, we have systematically explored MoS$_2$-MoX$_2$ heterostructure (see figure 1) within the framework of Density Functional Theory (DFT) using SIESTA code [8, 9].

COMPUTATIONAL DETAILS

In this work, we have used well tested Troullier Martin, norm conserving, relativistic pseudopotentials in fully separable Kleinman and Bylander form for Mo, S, Se and Te. The Generalized Gradient Approximation (GGA) according to the Perdew, Burke, Ernzerhof (PBE) parameterization has been used to treat electron-electron interaction. The interaction between adjacent layers is eliminated by introducing vacuum as large as of ~25 Å. A 250 Ry mesh cutoff has been used for the reciprocal space expansion of the total charge density. Brillion zone has been sampled by using 15×15×3 Monkhorst-Pack of k points. Localized atomic orbitals basis set has been used with confinement energy of 0.02 Ry. Optical calculations were carried out using 33x33x3 optical mesh and 0.2 eV optical broadening.
RESULTS AND DISCUSSIONS

Structural Properties

The calculated structural parameters, band gap and binding energy for MoS$_2$-MoX$_2$ heterostructures have been tabulated in table 1.

Calculated structural parameters for MoS$_2$-MoS$_2$ nanostructure are found to be in close agreement with the other reported values elsewhere [10, 11]. Our calculated results show that $d_{Mo-S}$ ($d_{Mo-X}$) bond length decreases(increases) when S is replaced by Se. A similar feature can be seen in bond angle ($\Theta$) parameter. However, increase in bond length and bond angle is found when S is replaced by Te. This might be due to large lattice mismatch at the interface of MoS$_2$ and MoTe$_2$ monolayers as compared to mismatch in MoS$_2$-MoSe$_2$ heterostructure. To ensure the stability of the MoS$_2$-MX$_2$ heterostructure, we have calculated the binding energy ($E_{BE}$) as

$$E_{BE} = E_{MoS_2-MoX_2} - E_{MoS_2} - E_{MoX_2}$$

Where $E_{MoS_2-MoX_2}$ is total energy of MoS$_2$-MX$_2$ heterostructure, $E_{MoS_2}$ and $E_{MoX_2}$ is the total energy of MoS$_2$ and MoX$_2$ monolayer units as obtained from converged SIESTA runs. The binding energy is found to be -0.04 eV for MoS$_2$ and MoSe$_2$ while for MoTe$_2$ it is found to be -0.03 eV. The small magnitude of $E_{BE}$ indicates the weak van der waal interaction between the constituent monolayers which are strong enough to hold them together.

Electronic Properties

The electronic band structures of MoS$_2$-MoX$_2$ heterostructures have been calculated along highly symmetric $\Gamma$-M-K-$\Gamma$ directions. A systematic decrease in band gap has been observed on changing chalcogen atoms from S to Te (figure 2). It is clear from figure 2 that the MoS$_2$-MoTe$_2$ heterostructure have some valance band and conduction band cross-over around the Fermi level that indicate the semiconductor-to-metal transition. Thus we can say that heterostructuring offers a platform to tailor the band gap according to their demand in electronic devices.
The right side of band structures in figure 2 shows the total and respective partial density of states (PDOS) for all the considered heterostructure. We can see that the peaks of PDOS above the Fermi energy are mainly due to Mo-4d and S-3p in all the heterostructures while peaks below the Fermi level comes from the Mo-4d and X-np orbital, where X= S, Se, Te and n=3, 4, 5 respectively. Thus PDOS analysis reveals that valance band maxima (VBM) and conduction band minima (CBM) are confined on different layers which essentially reduces the band gap.

Dielectric Properties

The study of the dielectric functions helps to give a better understanding of electronic structure which can suggest potential applications in opto-electronic devices and the semiconductor industry. Dielectric properties of materials having hexagonal symmetry can be calculated with electric vector E perpendicular as well as parallel to c-axis. Here we discuss the dielectric properties of MoS\textsubscript{2}-MoX\textsubscript{2} heterostructures with electric vector E perpendicular to c-axis.

<table>
<thead>
<tr>
<th>System/Parameter (MoS\textsubscript{2}-MoX\textsubscript{2})</th>
<th>d\textsubscript{Mo-S}</th>
<th>d\textsubscript{Mo-X}</th>
<th>Θ\textsubscript{S-Mo-S}</th>
<th>Θ\textsubscript{S-Mo-S}</th>
<th>Band Gap</th>
<th>Binding Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>MoS\textsubscript{2}-MoS\textsubscript{2}</td>
<td>2.44,</td>
<td>2.44</td>
<td>81.18</td>
<td>81.18</td>
<td>1.49, 1.52</td>
<td>-0.04</td>
</tr>
<tr>
<td>MoS\textsubscript{2}-MoSe\textsubscript{2}</td>
<td>2.42</td>
<td>2.55</td>
<td>79.18</td>
<td>81.10</td>
<td>0.60</td>
<td>-0.04</td>
</tr>
<tr>
<td>MoS\textsubscript{2}-MoTe\textsubscript{2}</td>
<td>2.49</td>
<td>2.73</td>
<td>76.00</td>
<td>88.18</td>
<td>0.00</td>
<td>-0.02</td>
</tr>
</tbody>
</table>

In figure 3, imaginary part of dielectric function (ε\textsubscript{2}), electron energy loss (EEL), plasmon energy, static dielectric constant (ε\textsubscript{s}) for MoS\textsubscript{2}-MoX\textsubscript{2} heterostructure and corresponding structure peaks are given in table 2.

<table>
<thead>
<tr>
<th>System/Property (MoS\textsubscript{2}-MoX\textsubscript{2})</th>
<th>ε\textsubscript{2}</th>
<th>EEL</th>
<th>Plasmon Energy</th>
<th>ε\textsubscript{s}</th>
</tr>
</thead>
<tbody>
<tr>
<td>MoS\textsubscript{2}-MoS\textsubscript{2}</td>
<td>2.78</td>
<td>8.18</td>
<td>8.16</td>
<td>6.16</td>
</tr>
<tr>
<td>MoS\textsubscript{2}-MoSe\textsubscript{2}</td>
<td>2.55</td>
<td>7.89</td>
<td>7.86</td>
<td>6.54</td>
</tr>
<tr>
<td>MoS\textsubscript{2}-MoTe\textsubscript{2}</td>
<td>2.40</td>
<td>7.20</td>
<td>7.21</td>
<td>8.19</td>
</tr>
</tbody>
</table>

It is evident from table 2 that imaginary part of dielectric function (ε\textsubscript{2}) of MoS\textsubscript{2}-MoX\textsubscript{2} heterostructure shows the shift in peaks towards lower energy region when X is changing from S to Te. The shift of 0.23 eV and 0.15 eV has been found as one goes from S to Se and Se to Te respectively. The EEL function is proportional to inverse of dielectric function which can be calculated as :
It is found that in EEL spectra of considered heterostructures there is shift in peak positions towards lower energy as compared MoS$_2$-MoS$_2$ nano structure, although the shift in the peaks are not uniform as can be seen in figure 3(b) and table 2. The shift of 0.29 eV and 0.69 eV have been observed with change of X from S to Se and Se to Te.

Real part of dielectric function ($\varepsilon_1$) is shown in figure 3(c), for considered heterostructures. It can be seen from figure 3(c) that the energy values at which the $\varepsilon_1$ crosses the zero axis from the negative side (marked by a pink oval) indicates the plasmonic excitations at these energies. These values are very close to peak energies in EEL as can be seen in table 2. Furthermore, the static dielectric constant has been investigated for heterostructures. Static dielectric constant ($\varepsilon_s$) is given by value of real part of dielectric function at zero frequency. Interestingly, the static dielectric constant increases with going from MoS$_2$-MoS$_2$ to MoS$_2$-MoTe$_2$ (table 2). The behavior is just opposite to the change in band gap (table 1). This can be understood within the framework of Penn model expression [12]

$$\varepsilon_1(0) = 1 + \left(\frac{\hbar \omega_p}{E_g}\right)^2,$$

in which static dielectric constant is inversely proportional to the band gap.

**Conclusions**

In conclusion, we have performed comparative first principle calculations to study the electronic and dielectric properties of MoS$_2$-MoX$_2$ heterostructure with X= S, Se, Te. We find a systematic decrease/increase in band gap/static dielectric constant is as X changes from S to Te. In dielectric response, shift in peaks positions have been observed. Our study reveals that MoS$_2$-MoX$_2$ heterostructures might be useful for various electronic and optoelectronic applications which may hold the key towards heterostructures based electronics.

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