First Principle Study for Optical Properties of TMDC/Graphene Heterostructures

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The transition-metal dichalcogenide (TMDC) in the family of MX$_2$ (M = Mo, W; X = S, Se) and the graphene (Gr) monolayer are an atomically thin semiconductor and a semimetal, respectively. The monolayer MX$_2$ has been discovered as a new class of semiconductors for electronics and optoelectronics applications. Because of the hexagonal lattice structure of both materials, MX$_2$ and Gr are often combined with each other to generate van der Waals heterostructures. Here, the MX$_2$/Gr heterostructures are investigated theoretically based on density functional theory (DFT). The electronic structure and the optical properties of four different MX$_2$/Gr heterostructures are computed. We systematically compare these MX$_2$/Gr heterostructures for their complex permittivity, absorption coefficient, reflectivity and refractive index.

I. INTRODUCTION

Materials in confined geometries are hosts to novel phenomena. For example, in one dimension (1D), the fractional charge excitation or the soliton is found in the electronic properties of the organic polyacetylene [1], and the Haldane conjecture [2], which corresponds to the electronic properties of the organic polyacetylene [1], and the Haldane conjecture [2], which corresponds to the electronic properties of the organic polyacetylene [1], and the Haldane conjecture [2], which corresponds to the electronic properties of the organic polyacetylene [1], and the Haldane conjecture [2], which corresponds to the electronic properties of the organic polyacetylene [1], and the Haldane conjecture [2], which corresponds to the electronic properties of the organic polyacetylene [1], and the Haldane conjecture [2], which corresponds to the electronic properties of the organic polyacetylene [1], and the Haldane conjecture [2], which corresponds to the electronic properties of the organic polyacetylene [1], and the Haldane conjecture [2], which corresponds to 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II. MATERIALS AND METHODS

The first-principles calculations are based on the local-density approximation (LDA) proposed by Kohn and Sham [72], which approximates the total energy of the multielectron system. The simulations were implemented using the software package NANOncal and its accom-

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The lattice mismatch ratios and the binding energies of the most stable configurations of MoS$_2$/BP, MoSe$_2$/BP, WS$_2$/BP and WSe$_2$/BP are $-196$ meV, $-130$ meV, $-201$ meV and $-141$ meV, respectively, \cite{32, 63}. As listed in Table I, all the binding energies for the MX$_2$/Gr heterostructures in this study are negative, and the values are close to MX$_2$/BP, demonstrating that the structural stability of MX$_2$/Gr is similar to that of MX$_2$/BP.

### III. RESULTS

#### A. Band structures

The direct band gaps of the MoS$_2$, MoSe$_2$, WS$_2$ and WSe$_2$ monolayers were 1.82 eV, 1.56 eV, 1.95 eV and 1.64 eV, respectively, \cite{36}, where both the conduction band minimum (CBM) and the valence band maximum (VBM) were at the K-point in the Brillouin zone. The Dirac point of the Gr was located at the K-point and pinned to the Fermi level. All the results of the energy band structures for the MX$_2$ monolayers are consistent with the existing literature \cite{17, 35}. Now we report the energy band structures and the electronic density of states (DOS) for the four MX$_2$/Gr, as shown in Figure 2. We found that the band structure of MX$_2$/Gr could basically be regarded as the overlap of the band struc-

| TABLE II. The optimized atom-atom distances as well as the MX$_2$ layer – Gr layer distances. |
|---------------------------------------------------------------|
| MX$_2$/Gr | Mo-S | Mo-C | S-C | C-C | MoS$_2$/Gr |
|-----------|------|------|-----|-----|------------|
| MoS$_2$/Gr | 2.404Å | 4.826Å | 3.089Å | 1.600Å | 2.973Å |
| MoSe$_2$/Gr | 2.349Å | 4.920Å | 3.270Å | 1.626Å | 3.161Å |
| WS$_2$/Gr | 2.379Å | 4.774Å | 3.078Å | 1.596Å | 2.954Å |
| WSe$_2$/Gr | 2.354Å | 4.940Å | 3.286Å | 1.625Å | 3.178Å |

The lattice constants of the MoS$_2$/Gr, MoSe$_2$/Gr, WS$_2$/Gr and WSe$_2$/Gr monolayers were 3.166 Å, 3.288 Å, 3.153 Å, 3.282 Å and 2.47 Å, respectively. For all the MX$_2$/Gr heterostructures, lattice mismatch ratios less than 5% were achieved by choosing a 3 x 3 MX$_2$ supercell and a 4 x 4 Gr supercell, as shown in Figure 1. The details of the lattice mismatch ratios are listed in Table I. After the structure optimization, the lattice contents were 9.666 Å, 9.854 Å, 9.648 Å and 9.845 Å for MoS$_2$/Gr, MoSe$_2$/Gr, WS$_2$/Gr and WSe$_2$/Gr, respectively. The details of the atom-atom distances as well as the MX$_2$ layer–Gr layer distances are listed in Table II. The total number of atoms in the simulations was 59 for MX$_2$/Gr, 27 for the 3 x 3 monolayer of MX$_2$, and 32 for the 4 x 4 monolayer of Gr.

The binding energies $E_b$ are calculated by the energy difference between the heterostructures and the monolayers:

$$E_b = E_{MX_2/Gr} - E_{MX_2} - E_{Gr},$$

where $E_{MX_2/Gr}$, $E_{MX_2}$ and $E_{Gr}$ are the total energies of the heterostructures, isolated MX$_2$ and Gr, respectively. It is interesting to compare other heterostructures, such as MX$_2$/BP \cite{59}, as regards binding energies. The interface binding energies of the most stable configurations of MoS$_2$/BP, MoSe$_2$/BP, WS$_2$/BP and WSe$_2$/BP are $-196$ meV, $-130$ meV, $-201$ meV and $-141$ meV, respectively, \cite{59}. As listed in Table I, all the binding energies for the MX$_2$/Gr heterostructures in this study are negative, and the values are close to MX$_2$/BP, demonstrating that the structural stability of MX$_2$/Gr is similar to that of MX$_2$/BP.

The lattice mismatch ratios and the binding energies of TMDCs/graphene with 3 x 3 supercell of MX$_2$ and 4 x 4 supercell of graphene are

| MX$_2$/Gr | MoS$_2$/Gr | MoSe$_2$/Gr | WS$_2$/Gr | WSe$_2$/Gr |
|-----------|------------|------------|----------|------------|
| mismatch ratio | 1.83% | 0.10% | 2.04% | 0.01% |
| $E_b$ | $-194$ meV | $-146$ meV | $-178$ meV | $-246$ meV |

FIG. 1. The stacking of the 3 x 3 MoS$_2$ supercell and the 4 x 4 Gr supercell. (a) The side view. (b) The top view. For the other MX$_2$/Gr, the atom–atom distances are listed in Table II.

panning software packages DEVICESTUDIO and OPTIC- CAL \cite{73, 74}. A plane wave basis was set with a cutoff energy of 80 Hartree and a 5 x 5 x 1 Γ-centered k-points grid. The atomic structures were relaxed until the force was smaller than 0.03 eV/Å and the total energy convergence criterion was set as $10^{-4}$ eV. In order to avoid interactions in the vertical direction between neighboring slabs, a vacuum layer of 24 Å was added between different slabs.

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| mismatch ratio | 1.83% | 0.10% | 2.04% | 0.01% |
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FIG. 2. The energy band structures and the DOS for the MX$_2$/Gr van der Waals heterostructures. The partial DOS values are labeled with s, p, or d, corresponding to the orbital contributions, and the total DOS is labeled with T. (a,b) MoS$_2$, (c,d) MoSe$_2$, (e,f) WS$_2$, (g,h) WSe$_2$.

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The Schottky contacts are formed between the semiconducting MX$_2$ and the metallic Gr. The Schottky barrier is one of the most important characteristics of a semiconductor–metal junction and dominates the transport properties. Based on the Schottky–Mott model [75–77], at the interface of the metal and semiconductor, an n-type Schottky barrier height (SBH) $\Phi_{Bn}$ is defined as the energy difference between the Fermi level $E_F$ and the conduction band minimum $E_C$, i.e., $\Phi_{Bn} = E_C - E_F$. Similarly, the p-type SBH $\Phi_{Bp}$ is defined as the energy difference between $E_F$ and the valence band maximum $E_V$, i.e., $\Phi_{Bp} = E_F - E_V$. The n/p-type Schottky contacts are classified by the smaller SBH. The SBH are $\Phi_{Bn} = 0.29$ eV and $\Phi_{Bp} = 1.23$ eV for MoS$_2$/Gr, $\Phi_{Bn} = 0.75$ eV and $\Phi_{Bp} = 0.65$ eV for MoSe$_2$/Gr, $\Phi_{Bn} = 0.39$ eV and $\Phi_{Bp} = 1.13$ eV for WS$_2$/Gr, and $\Phi_{Bn} = 1.00$ eV and $\Phi_{Bp} = 0.61$ eV for WSe$_2$/Gr, respectively. Therefore, MoS$_2$/Gr, MoSe$_2$/Gr, WS$_2$/Gr and WSe$_2$/Gr are the n-type, p-type, n-type and p-type Schottky contacts, respectively.

B. Optical properties

In order to understand the optical properties, the complex permittivity or the so-called dielectric function was computed under the long-wave approximation, i.e., $\vec{q} = 0$. The complex permittivity $\varepsilon(\omega) = \varepsilon_{\text{real}}(\omega) + i\varepsilon_{\text{imag}}(\omega)$ as...
FIG. 3. The complex permittivities for MX\textsubscript{2}/Gr heterostructures and MX\textsubscript{2} and Gr monolayers as functions of incident photon energy. (a),(c) The real part of the permittivity $\varepsilon_{\text{real}}$. (b),(d) The imaginary part of the permittivity $\varepsilon_{\text{imag}}$.

a function of incident photon energy is [78]

$$\varepsilon(\omega) = 1 + \frac{2e^2}{\varepsilon_0 m^2 V} \sum_{\alpha\beta} \left| \langle \psi_{\beta} | \hat{\varepsilon} \cdot \hat{p} | \psi_{\alpha} \rangle \right|^2 \frac{f(E_{\alpha}) - f(E_{\beta})}{(E_{\beta} - E_{\alpha})^2 / \hbar^2 E_{\beta} - E_{\alpha} - \hbar \omega - i\eta}$$

(2)

where $e$ is the electron charge, $\varepsilon_0$ is the vacuum permittivity, $m$ is the electron mass, $\hat{\varepsilon}$ is the direction of the vector potential, $\hat{p}$ is the momentum operator, $\hbar \omega$ is the photon energy, and $f(E_{\alpha})$ and $f(E_{\beta})$ are the Fermi–Dirac distribution functions. Since $\varepsilon = n^2$, i.e., $\varepsilon_{\text{real}} + i\varepsilon_{\text{imag}} = (n + i\kappa)^2$, the refraction index $n$ and the extinction coefficient $\kappa$ are obtained:

$$n^2 = \frac{|\varepsilon| + \varepsilon_{\text{real}}}{2},$$

(3)

$$\kappa^2 = \frac{|\varepsilon| - \varepsilon_{\text{real}}}{2}.$$  

(4)

The real part $\varepsilon_{\text{real}}$ is caused by various kinds of displacement polarization inside the material and represents the energy storage term of the material. The imaginary part $\varepsilon_{\text{imag}}$ is related to the absorption of the material, including gain and loss. Therefore, the permittivity must be real in the absence of the incident photon energy, i.e., $\varepsilon(\omega = 0) = \varepsilon_{\text{real}}$. It is expected that the smaller the energy gap of a material, the larger its $\varepsilon(0)$. On the other hand, since the DOS only appears in a finite range of energy in the numerical simulation, electron transitions by the absorption of photons do not occur if the photon energy is too large. Therefore, without photon absorption the computed $\varepsilon_{\text{imag}}$ is close to zero in the large limit of the incident photon energy, and the permittivity approaches a constant real value.

In Figure 3, we show the real part and the imaginary part of the complex permittivity for MX\textsubscript{2}/Gr heterostructures and MX\textsubscript{2} and Gr monolayers. Since the energies corresponding to the peak positions of the DOS in the conduction and valence bands of the MX\textsubscript{2}/Gr were smaller than those of MX\textsubscript{2}, the peak positions of the real part $\varepsilon_{\text{real}}(\omega)$ of MX\textsubscript{2}/Gr in Fig. 3(c) had a red shift compared with the MX\textsubscript{2} in Fig. 3(a). The highest peak corresponding energy of the imaginary part $\varepsilon_{\text{imag}}(\omega)$ of the MX\textsubscript{2}/Gr in Fig. 3(d) was about 0.8 eV to 0.9 eV, which corresponds to the position where the real part decreases the fastest.

After obtaining the dielectric function, the absorption coefficient $\alpha$ is computed by

$$\alpha = \frac{2\omega\kappa}{c},$$

(5)

and the reflectivity $R$ is

$$R = \frac{(n - 1)^2 + \kappa^2}{(n + 1)^2 + \kappa^2}.$$  

(6)

Figure 4 compares MX\textsubscript{2}/Gr, MX\textsubscript{2} and Gr for their absorption coefficient $\alpha$, reflectivity $R$ and refractive index $n$. Since MX\textsubscript{2}/Gr has a smaller optical band gap
FIG. 4. The comparison of MX$_2$/Gr heterostructures and MX$_2$ and Gr monolayers according to their (a),(d) absorption coefficient $\alpha$, (b),(e) reflectivity $R$ and (c),(f) refractive index $n$. The rainbow bars represent the energy range of visible light, from 1.59 eV to 3.26 eV.

compared with the MX$_2$ monolayer, MX$_2$/Gr has a wider range of light absorption, from 0.6 eV to 4 eV. As shown in Fig. 4(b),(e), MX$_2$/Gr had a higher reflectivity than MX$_2$ in the infrared area ($\hbar\omega < 1.2$ eV), and had a higher reflectivity than Gr in the visible light area. We compare the real part of the permittivity of monolayer MX$_2$ in Fig. 3(a) with the refractive index of monolayer MX$_2$ in Fig. 4(c), and compare the real part of the permittivity of the MX$_2$/Gr heterostructure in Fig. 3(c) with that of MX$_2$/Gr in Fig. 4(f). It was found that the changing trends from Fig. 3(a) to Fig. 4(c) are similar to those from Fig. 3(c) to Fig. 4(f). This means that the real part of the dielectric constant dominates the effect of the refractive index. The above simulation results suggest that MX$_2$/Gr heterostructures are good candidate materials for optical applications.

IV. DISCUSSION

Two-dimensional heterostructures based on TMDCs exhibit the enhancement of electrical and optoelectrical properties, which are promising for next-generation optoelectronics devices. We systematically computed the complex permittivity $\varepsilon(\omega)$, absorption coefficient $\alpha(\omega)$, reflectivity $R(\omega)$ and refractive index $n(\omega)$ for MX$_2$/Gr heterostructures, where $M = $ Mo, W; and $X = $ S, Se. Our results qualitatively agree with those from previous studies on MoS$_2$/Gr [69] and WSe$_2$/Gr [70], where red shifts in the $\alpha(\omega)$, $R(\omega)$ and $n(\omega)$ were found compared with MoS$_2$ and WSe$_2$ monolayers. We extended the investigations to other MX$_2$/Gr heterostructures, and found qualitatively similar behavior in their optical properties.

It is worth comparing our MX$_2$/Gr results with the recent simulation results on the MX$_2$/BP in terms of absorption abilities [59]. Although different types of van der Waals heterostructures were found in MX$_2$/BP (type-I for MoS$_2$/BP and WS$_2$/BP; type-II for MoSe$_2$/BP and WSe$_2$/BP), all the materials of MX$_2$/BP have excellent absorption abilities in the infrared and visible light range, i.e., $\alpha(\omega) \approx 0.01$ nm$^{-1}$ to 0.05 nm$^{-1}$ for the wavelength $400$ nm $\leq \lambda \leq 1200$ nm [59]. In our study, all the MX$_2$/Gr were type-I heterostructures, and the values of the absorption coefficients were in the same range compared with MX$_2$/BP in the infrared and visible light range. Therefore, MX$_2$/Gr can be utilized as alternative materials for the applications of solar optoelectronics devices.

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