



First-principles determination of electronic properties of MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂ vdW heterostructures on mica with spin-orbit coupling

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ABSTRACT

In this study, Density functional theory (DFT) calculations were conducted to calculate the structural, electronic, transport, and optical properties of MoSe₂ and HfSe₂ monolayers (MLs) and the proposed modelled interfaces of MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂ on mica substrate. According to atomistic calculations, in MoSe₂/HfSe₂/mica, the mica substrate acts as the important source of excess charge that dopes the adjacent 2D TMDs layers, while by adding another layer of MoSe₂ to the interface, the HOMO and LUMO states showed more charge delocalization between MoSe₂ and HfSe₂ MLs. The Band structure calculation reveal that the indirect band gaps with spin-orbit coupling (SOC) calculations have estimated to be 0.43 eV /0.31 eV and 0.37 eV/0.24 eV from K→K/T→K for MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂ van der Waals (vdW) heterostructures, respectively, lower than the band gaps of MoSe₂ (1.44 eV)/HfSe₂ (1.20 eV) nanosheets. Mulliken charge analysis indicated how presence the MoSe₂ monolayer able to influence Se atoms in centre of the MoSe₂/HfSe₂/MoSe₂ to receive the charge, while in MoSe₂/HfSe₂ those situated in the side of MoSe₂ participated in the charge transfer more. Our results point to the phonon-limited mobility of 52.1 cm² V⁻¹s⁻¹ with a carrier density of 2.91 × 10¹² cm⁻³ for MoSe₂/HfSe₂/MoSe₂ interface, which is higher than that of HfSe₂ but lower compared to what was previously found for the MoSe₂ monolayer. We have also computed a very low lattice thermal conductivity of 0.58 Js⁻¹m⁻¹K⁻¹ for the MoSe₂/HfSe₂/MoSe₂ heterostructure is mainly provided by an in-plane (yy) tensor with a value of 0.401 Js⁻¹m⁻¹K⁻¹. Moreover, the optical properties showed a remarkable improvement in the absorption coefficient of vdW heterostructures than MLs with the first adsorption peaks at 12 THz and 36 THz. The DFT outcomes revealed how adding the second layer of MoSe₂ in MoSe₂/HfSe₂/MoSe₂ can change the adsorption intensity and dielectric constant along the different in-plane directions as well as interlayer coupling.

1. Introduction

Ultrathin two-dimensional (2D) of transition metal dichalcogenides (TMDs) are fundamentally intriguing materials and represent an alternative group of 2D layered structures with different properties than metallic graphene. The features of TMDs can be tailored depending on their crystalline structure, composition, number and stacking sequence of layers and dimensions [1,2]. Moreover, their tunable electronic structure makes them attractive for use in various applications such as in electrode materials for supercapacitors [3], photoluminescence [4], and

optoelectronic devices [5,6].

MoSe₂'s structure as a TMD has been extensively studied, and its remarkable potential for use in nanoelectronics has been demonstrated by the use of field-effect transistors (FET) [7,8]. This structure shows low carrier mobility, proven by experiments (50–160 cm²v⁻¹s⁻¹) [9] and DFT calculations (240 cm²v⁻¹s⁻¹) [10], if compared to some semiconductors like silicon (<1400 cm² V⁻¹s⁻¹) [11] and Germanium (2800 cm² V⁻¹s⁻¹) [12]. On the other hand, monolayer HfSe₂ with a crystal structure similar to Si [13] showed very different theoretical and experimental mobility values. A theoretical study by Zhang et al. [10]

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based on DFT predicted a remarkably high phonon-limited mobility of $3500 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ at room temperature for this monolayer. Still, a later study of density functional perturbation theory in conjunction with the Boltzmann transport equation showed good agreement with the experimental value of $0.3\text{--}6.3 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ [14]. The band gap of a MoSe_2 monolayer without spin-orbit coupling (SOC) is typically a direct band gap of around $1.4\text{--}1.6 \text{ eV}$, while the introduction of SOC significantly affects its electronic band structure by a direct band gap of $\sim 1.35 \text{ eV}$ [15–17]. The calculated band gaps for monolayer HfSe_2 with and without SOC significantly depended on the theoretical method used, however, the values show the band gaps of $0.7\text{--}0.9 \text{ eV}$ (without SOC) and slightly lower as 0.6 eV (with SOC), with experimental reports suggesting a gap of about 1.0 eV [18–20].

So far, the layering of the same or different types of materials with a vacuum in between has been explored, and shown to be significantly impact band alignment, hole and electron mobility, binding energy, thermoelectric characteristics, and optical properties. The interfaces of 2D TMDs materials with similar crystal structures but different electronic band structure properties permit the formation of van der Waals (vdW) heteroepitaxial materials, offering a variety of band alignments, and representing a new platform with desirable novel functionality exploitable in the area of electronics and optoelectronics [21–25]. According to an experimental and theoretical study by Aretouli et al. [26], an interesting band diagram can be found in $\text{MoSe}_2/\text{HfSe}_2$. In this study, using molecular beam epitaxy, atomically thin 2D semiconductor $\text{MoSe}_2/\text{HfSe}_2$ vdW heterostructure is grown on $\text{AlN}(0001)/\text{Si}(111)$ substrates. Experimental measurements using in-situ angle-resolved photoelectron spectroscopy (ARPES) indicate a small valence band offset of approximately 0.13 eV at the $\text{MoSe}_2/\text{HfSe}_2$ heterointerface. The band alignments at the $\text{MoSe}_2/\text{HfSe}_2$ confirm a type II band alignment in a $p\text{--}n$ heterojunction configuration, with prospective applications in (opto-)electronics. In another study, Wang et al. [27] have prepared 2D $\text{MoSe}_2/\text{WSe}_2$ vertical and lateral heterostructures by using Chemical Vapor Deposition (CVD) and a combination of Physical Vapor Deposition (PVD) and CVD, respectively. Subsequently, the structure, electronic and optoelectronic properties of these two types of heterostructures were characterized. The results indicate that FET based on single-layer $\text{MoSe}_2/\text{WSe}_2$ lateral heterostructures, and single-layer WSe_2 /multi-layer MoSe_2 and single-layer MoSe_2 /multi-layer WSe_2 vertical heterostructures exhibit significant rectification effects. In a similar work, Li et al. [28] indicated the potential utility of a vertical stack consisting of monolayers of $\text{MoSe}_2/\text{WTe}_2$ semiconductors for application in a tunneling FET. The simulation results suggest that the Thin-TFETs can achieve very steep subthreshold swing, the lower limit of which is ultimately set by the band tails in the energy gaps of the 2D materials produced by energy broadening. A comprehensive interface study has been performed for $\text{WSe}_2/\text{HfSe}_2$, revealing a band gap from the K-point to the M-point with a value of 0.21 eV in this heterostructure. The authors explained that the optical absorption intensity of the $\text{WSe}_2/\text{HfSe}_2$ vdW heterostructure can reach the order of 10^5 [29].

Beyond the aforementioned points, in this study, we will focus on how to enhance the electronic transport and optical properties of the MoSe_2 and HfSe_2 structures for application in low-frequency THz amplification (with a frequency range of $0.1\text{--}5 \text{ THz}$) by constructing MoSe_2 and HfSe_2 heterostructure systems. Terahertz waves (wavelengths $0.03\text{--}3 \text{ mm}$), occupy the transition region between microwave (radio) and infrared (optical) radiation. Because this band bridges the gap between electronics (classical, low-frequency) and photonics (quantum, high-frequency), it possesses unique dual characteristics that make it valuable for scientific and industrial applications. Furthermore, THz technology demonstrates broad application prospects in multiple cutting-edge fields, including biomedical imaging, security inspection, 6G communications, and materials science [30–32]. The main challenges and development directions of THz technology lie in realizing its potential faces significant bottlenecks, often referred to as the "terahertz gap"—the lack of efficient, compact, and affordable sources and

detectors [33,34]. In this context, exploring emerging materials, such as 2D heterostructures, and integration methods, is attracting increasing attention. Following our previous studies regarding the THz properties in 2D TMDs materials, such as SnSe_2 and SnSe [24,35], VSe_2 [25], and WSe_2 [36], and graphene [37,38], this research involves several aspects.

In this paper, we proposed two interfaces of $\text{MoSe}_2/\text{HfSe}_2$ and $\text{MoSe}_2/\text{HfSe}_2/\text{MoSe}_2$ modelled on the mica ($\text{KAl}_2(\text{AlSi}_3\text{O}_{10})(\text{OH})_2$) as the substrate. The choice of the mica comes from the experimental studies which have reported that MoSe_2 on HfSe_2 vdW heterostructures on mica substrates represent unique band alignments and the high-quality interface provided by the mica's atomic flatness. These structures typically form weak type-II $p\text{--}n$ heterojunctions, facilitating efficient charge separation and making them suitable for applications like photodetectors and TFETs. The substrate advantages of mica are because of its atomic smoothness (roughness $\sim 0.053 \text{ nm}$) and chemical inertness. It allows for vdW epitaxy, which enables the growth of high-quality, large-area crystalline layers like MoSe_2 with minimal strain despite lattice mismatches. The fabrication methods are Molecular Beam Epitaxy (MBE) which often used to grow epitaxial HfSe_2 and $\text{MoSe}_2/\text{HfSe}_2$ layers with high precision and CVD where frequently employed for large-area synthesis of MoSe_2 on mica by the salinization of precursor films [26,39–42].

A comprehensive theoretical insight into the electronic structures, charge transfer, transport features such as mobility, carrier concentration and thermal conductivity as well as optical properties have been studied. Here, the following main issues are considered: (I) the band structure and projected densities of states (PDOS) calculations for the MLs of MoSe_2 , HfSe_2 , $\text{MoSe}_2/\text{HfSe}_2/\text{mica}$ and $\text{MoSe}_2/\text{HfSe}_2/\text{MoSe}_2/\text{mica}$ will be evaluated; the atomistic calculations have discussed the effect of SOC calculations in the band gap values and the position of the valence and conduction bands along the high-symmetry points in the reciprocal space. (II) the molecular energy spectrum and HOMO (Highest Occupied Molecular Orbital)–LUMO (Lowest Unoccupied Molecular Orbital) energy levels and isosurfaces have been simulated, (III) the charge transfer with reference to the Mulliken charge calculations are determined for the monolayers as well as the interfaces; (IV) the electronic transport coefficients of $\text{MoSe}_2/\text{HfSe}_2$ and $\text{MoSe}_2/\text{HfSe}_2/\text{MoSe}_2$ interfaced systems will be sought; (V) the optical properties of the monolayers and $\text{MoSe}_2/\text{HfSe}_2$ and $\text{MoSe}_2/\text{HfSe}_2/\text{MoSe}_2$ heterostructure in the THz range will be considered.

2. Computational Details

The Density Functional Theory (DFT) calculations were carried out using the Quantum ATK (QATK) [43] software, which was used to simulate and characterize the properties of different materials and devices [44–47]. The Kohn–Sham (KS) formulation [48,49] were resolved within the framework of the linear combinations of atomic orbitals (LCAO) basic set [50]. Norm-conserving (NC) PseudoDojo pseudopotentials (PPs) were adopted [51] to describe the valence orbitals approximating the core electrons. We performed the complete optimization of the cells' volumes, shapes, and atomic positions on the free-standing and heterostructure systems employing Generalized Gradient Approximation (GGA) and the Perdew–Burke–Ernzerhof (PBE) functional [52,53]. Numerical experiments have been carried out with the inclusion of dispersion corrections and employing the Grimme method (PBE-D3) [54]. For atomic relaxation and band structure calculations, we used k -points mesh $12 \times 12 \times 1$ grids for the monolayered and interfaced systems. The band structure was calculated using a symmetrical line in the $\Gamma\text{--}M\text{--}K\text{--}\Gamma$ direction in reciprocal space. Structural optimization was carried out until the residual forces fell below $0.001 \text{ eV/\text{Å}}$. The electronic convergence tolerance was set to 10^{-5} eV . For all calculations, a kinetic energy cutoff of 120 Ry was chosen for the integration mesh.

Since SOC calculation is fundamental to many phenomena in solid-state physics, by providing essential insights into the process of

extracting the spin interactions from the underlying electronic structure obtained from first-principles calculations [55–57], in this study, the calculations including SOC have been performed with fully relativistic PPs and a noncollinear representation of the electronic spin degrees of freedom. So, we applied the noncollinear spin-orbit with SOGGA exchange-correlation and PseudoDojo-SO PPs to perform the SOC field. As discussed later, SOC calculations in both monolayers and their vdW heterostructure enable more overlapping the neighboring wavefunctions and changing the energy of the valence band edge (VBE) and conduction band edge (CBE) along the high-symmetry points in the Brillouin zone (Bz) [58]. The completely relativistic Ultra basis set has been used for every element, pointing out that in this basis set there are more pseudo-atomic orbitals.

In computational physics, SOC and hybrid Heyd-Scuseria-Ernzerhof (HSE06) functionals solve entirely different problems of the materials property. HSE06 screened hybrid functional effectively corrects the systematic band gap underestimation seen in local density approximation (LDA) or generalized gradient approximation (GGA) by introducing a portion of exact Fock (Hartree-Fock) exchange [59,60]. In the other side, SOC splits the degenerate bands into spin-up and spin-down states, correcting band shapes and enabling spin-valley physics. It adjusts the position of the Valence Band Maximum (VBM) and the Conduction band minimum (CBM), however, generally does not correct the overall band gap size significantly on its own. For the most accurate electronic structure of both interfaces of MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂, the ideal approach is combining both methods HSE + SOC. This captures both the correct fundamental band gap energy (HSE06) and the spin-split band characteristics (SOC).

QuantumATK provides the possibility to use HSE06 + SOC, but there are important software limitations and setup requirements. Since LCAO basic set has been used, by choosing HSE06 calculations, the LCAO calculator automatically revert to unpolarized configurations. This means that it's not possible to use the full noncollinear calculations with hybrid functionals natively. Indeed, SOGGA can absolutely use with fully relativistic pseudopotentials and a noncollinear representation. It worthies to notice that calculating the properties of TMDs requires the inclusion of SOC because these materials—like MoSe₂, WS₂, HfSe₂ and WSe₂ exhibit strong relativistic effects. MoSe₂ and HfSe₂ materials have heavy metals with atomic number ($Z \approx 42$) for Mo, ($Z \approx 72$) for Hf, ($Z \approx 34$) for Se, generate a massive effective internal effective magnetic field experienced by moving electrons due to relativistic effects. Previous theoretical studies have showed that combining SOC with the GGA captures these relativistic phenomena, resolving key degeneracies and accurately mapping valleys in the Brillouin zone [61–65].

To analyse the energy levels of HOMO-LUMO of MoSe₂/HfSe₂/mica and MoSe₂/HfSe₂/MoSe₂/mica, molecular projected self-consistent Hamiltonian (MPSH) calculations was executed. The electronic transport properties of the interfaced system including phonon-limited mobility, carrier concentration, and thermal conductivity responses were calculated using the Boltzmann transport equation (BTE). The mobility (μ) calculations can be applied to the conductivity (σ) via,

$$\mu = \frac{\sigma}{ne} \quad (1)$$

where n is the carrier density and e is the electronic charge [66]. To this aim, we computed the dynamical matrix by setting the number of repetitions to $7 \times 7 \times 1$ for $n_A \times n_B \times n_C$. The same number of repetitions has been used to compute Hamiltonian derivatives. Then, the following steps of the electron-phonon couplings and mobility calculations have been estimated with high k-points of $20 \times 20 \times 1$ grids to evaluate the transport properties at of MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂ at 300° K.

The real part of the dielectric function ($\text{Re}(\omega)$) relates to the material's refractive index (n), while its imaginary part ($\text{Im}(\omega)$) relates to the extinction coefficient (κ), also known as the absorption coefficient (α), and together these form the complex n calculated by the following

Formula [67,68]

$$\alpha_a = 2 \frac{\omega}{c} \kappa \quad (2)$$

$$n = \sqrt{\frac{\sqrt{\text{Re}(\omega)^2 + \text{Im}(\omega)^2} + \text{Re}(\omega)}{2}} \quad (3)$$

$$\kappa = \sqrt{\frac{\sqrt{\text{Re}(\omega)^2 + \text{Im}(\omega)^2} - \text{Re}(\omega)}{2}} \quad (4)$$

The imaginary part of the n (defined also as the κ) is related to the absorption term of electromagnetic waves as they travel through a material.

And the term n is related to the complex relative permittivity (ϵ_r) through,

$$n + i\kappa = \sqrt{\epsilon_r} \quad (5)$$

3. Results and discussion

3.1. Structural parameters and electronic properties of the MoSe₂ and HfSe₂ nanosheets

Monolayers of MoSe₂ and HfSe₂ belong to the hexagonal lattice system, with space groups $P6_3/mmc$ and $P3\bar{1}m1$, respectively. These structures constitute the top and bottom Se layers sandwiching Mo (Hf) layers. In multilayer arrangements, layers are stacked together with the weak vdW interactions between Se atoms [69]–[70] (Fig. 1). After the full optimization of the MLs systems, the lattice constant of the monolayer MoSe₂ was optimized, and we obtained the parameters of $a = b = 3.28$ Å with a c-axis of the vacuum layer of 15 Å. The average bond length of Mo–Se is 2.53 Å. The corresponding lattice parameter of HfSe₂ is 3.76 Å [26], and the Hf–Se bond is 2.69 Å. Compared with the unit cell parameters optimized with the experimental data, there is little difference in the MoSe₂ structure, while the HfSe₂ structure showed a good consistency [71–73].

The band structures calculations of the MLs have been calculated, as seen in Fig. 1, along the high-symmetry k-points of Γ -M-K- Γ in the reciprocal space. The k-points location in the first Bz for the unit cell structure are: Γ (0, 0, 0), M (0, 0.5, 0) and K (0.333, 0.333, 0). Based on the calculations including SOC field, the predicted direct/indirect band gaps of MoSe₂ and HfSe₂ are 1.44 eV(K→K) and 0.59 eV(Γ →M), respectively. Inspection of data in Fig. 1 reveal that the effect of combining the DFT calculations with simulations based on effective realistic Hamiltonians of the spin-orbit physics in 2D TMDs materials. According to data predicted by SOGGA, the primary effect of SOC in monolayer MoSe₂ is the splitting of the VBE top at the K-point. This splitting has a strong spin-orbit effect and can increase the energy gap between the spin-polarized VBEs. However, SOC itself didn't directly transform an indirect bandgap material into a direct one or vice versa. Instead, it contributes to the energy levels and spin polarization near the band edge without fundamentally changing the direct-to-indirect bandgap character. As considered by the previous studies, the transition to an indirect bandgap or changes in the direct and indirect gap sizes are more strongly influenced by external factors like electric fields or strain, not the inherent SOC effect, which primarily causes band splitting rather than a complete shift from direct to indirect character [74–76]. About the HfSe₂ monolayer, SOC has strongly affected the VBE and CBE by lifting the spin degeneracy of electronic bands and causing energy shifts, which alters the magnitude of both direct and indirect band gap values.

According to our data analysis, we believe that SOGGA functional for the MLs systems are appropriate, since the band gaps we computed for MoSe₂ and HfSe₂ are in good agreement with those in previous experimental and theoretical studies [15,17–19,73,77]. The results reveal that

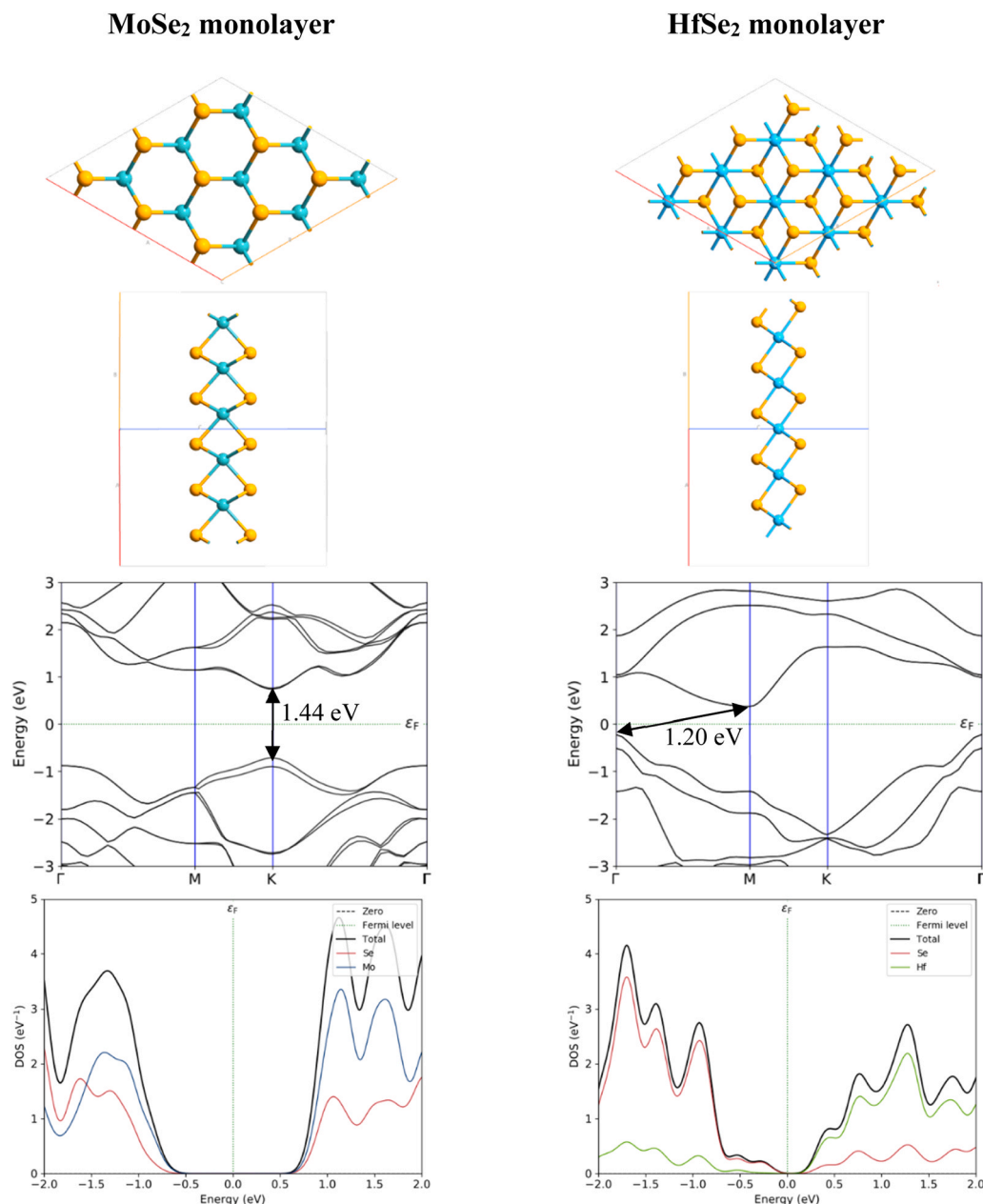


Fig. 1. The modeled structures of the MLs MoSe₂ and HfSe₂; the dark-blue, gold, and light-blue sticks are the Mo, Se, and Hf atoms, respectively. The corresponding band structure and PDOS calculations plots including SOC calculations along the high-symmetry directions in their first Bz.

to prediction the bandgap, conventional methodologies not necessarily always underestimate the bandgap of the semiconductors, while using Heyd-Scuseria-Ernzerhof functional (HSE06) hybrid functional and Many-Body Perturbation Theory (MBPT) methods such as GW are high-cost and time-consuming. It is worthy to notice that our previous study to evaluate the band structure calculations for SnSe and SnSe₂ monolayers confirmed that GGA and MGGA provided more accurate band gaps better than a specific hybrid [24].

Fig. 2 shows the absorption spectra for the material systems of MoSe₂ and HfSe₂, in the range of frequency of 0–400 THz. The atomistic calculations were computed along the *xx*-, *yy*- (in-plane), and *zz*-direction (out-of-plane) polarizations. The results show that while the MLs possess a weak absorption capacity at specific frequency ranges, the light absorption efficiency notably increases upon interface formation. The first approximated peaks of adsorption spectra are 65000 cm⁻¹ and 69000 cm⁻¹ at 388 THz and 315 THz, corresponding to MoSe₂ and HfSe₂ along the in-plane direction, respectively. As shown in Fig. 2, the

Re(ω) were calculated to be 7.38 and 4.05 for the MoSe₂ ML along the in-plane and out-of-plane polarizations, respectively, while corresponding values of 6.10 and 2.90 were predicted for HfSe₂ in the same directions. Moreover, the *Im*(ω) part reveal that the corresponding optical band gap of 355 THz and 308 THz for MoSe₂ and HfSe₂, respectively.

3.2. MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂ vdW heterostructure on mica

After consideration of the properties of individual MoSe₂ and HfSe₂ MLs, we simulated MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂ heterostructures on mica substrate. We focused on issues related to their vdW interactions employing structural and physical characterization using first principles calculations. It should be emphasis that for the first interface, the direct order of MoSe₂/HfSe₂/mica should be respected because from the experimental point of view, MoSe₂ is much more stable

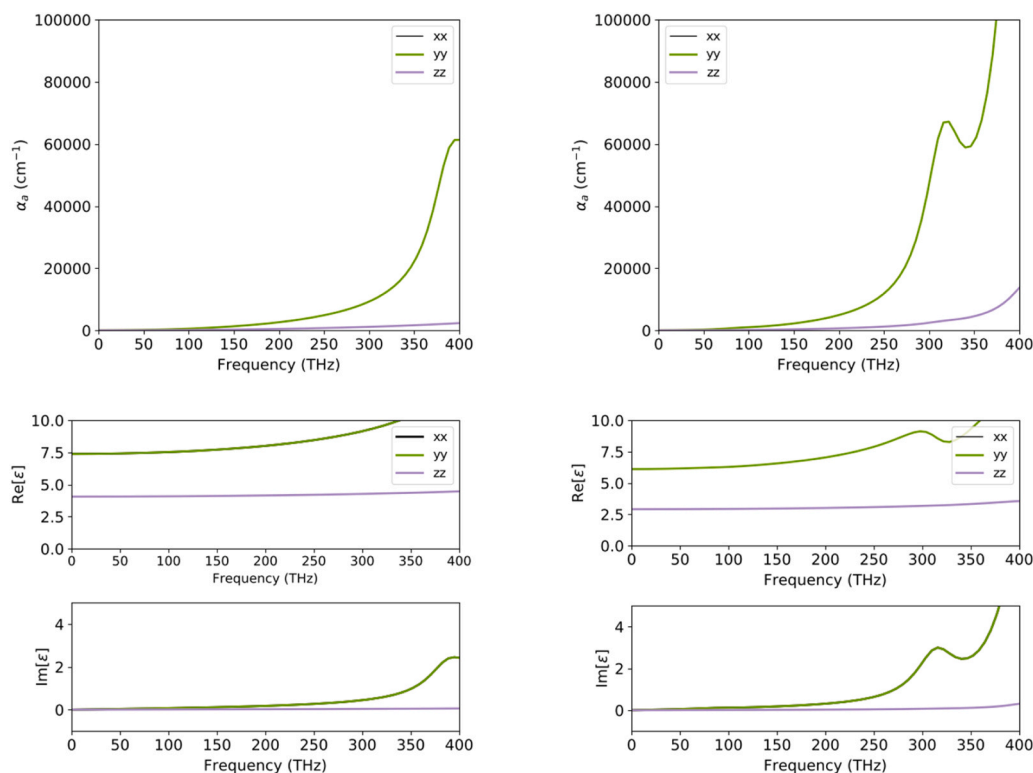


Fig. 2. The optical adsorption and imaginary and real part of dielectric constants of the monolayers MoSe₂ and HfSe₂ up to 400 THz frequency range.

in air against oxidation compared to HfSe₂ and essentially serves as a protective cap during processing of the bilayer for device fabrication [26,78,79]. According to Fig. 3, the cell dimensions of the heterostructures are $a = b = 13.15$ Å with $c = 52.03$ Å for MoSe₂/HfSe₂/mica and 55.24 Å for MoSe₂/HfSe₂/MoSe₂/mica. The size of the superlattices was specifically chosen to be large enough to avoid any interaction between the neighbouring layers. The results show that both interfaces on mica are vdW heterostructures which is characterized by weak coupling between the substrate and the TMDs layers, or between different 2D layers. The minimum vertical distances between the mica-HfSe₂ and MoSe₂-HfSe₂ are 3.38 Å and 3.65 Å in MoSe₂/HfSe₂/mica, respectively, while the corresponding values for MoSe₂/HfSe₂/MoSe₂/mica are 3.67 Å (mica-MoSe₂) and 3.49 Å (MoSe₂-HfSe₂).

The mica substrate has removed after the interfaces relaxing process to have highly efficient of isolating TMDs interactions. Cutting away the mica ensures that the band structures, density of states (DOS), charge transfer, and mobility metrics purely reflect the MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂ vdW interfaces rather than the mica's electrostatic influence or dangling bonds [80]. It worthies to mentioned that we run a single-point (SCF) energy calculation immediately after deleting the substrate, using the exact atomic coordinates from the relaxed

heterostructure. This gives the frozen electronic structure of the interfaces as it exists on the substrate. This method has already employed in the first-principles simulations for the interfaces [81].

To evaluate the systems stability, the interlayer binding energy (E_B) of the MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂ superlattices has been calculated as Eqs. 6 and 7 [82],

$$E_B = \frac{E(\text{MoSe}_2/\text{HfSe}_2) - E(\text{HfSe}_2) - E(\text{MoSe}_2)}{N} \quad (6)$$

$$E_B = \frac{E(\text{MoSe}_2/\text{HfSe}_2/\text{MoSe}_2) - E(\text{HfSe}_2) - 2E(\text{MoSe}_2)}{N} \quad (7)$$

where $E(\text{MoSe}_2/\text{HfSe}_2)$ and $E(\text{MoSe}_2/\text{HfSe}_2/\text{MoSe}_2)$ refer to total energy of superlattices, $E(\text{HfSe}_2)$ and $E(\text{MoSe}_2)$ are the total energy of the material monolayers, and N is the numbers of atoms in the supercells. The calculated E_B has obtained to be -12.8 meV and -14.2 meV for MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂, respectively, shows the latest structure is more stable.

The HOMO-LUMO band gap and isosurfaces from MPSH calculations have been demonstrated in Fig. 4. It has been predicted a higher HOMO-LUMO band gap when HfSe₂ ML has sandwiched between the MoSe₂ layers with 1.85 eV than the smaller value of 1.73 eV for MoSe₂/HfSe₂/mica. In comparison, the HOMO energy value a bit decreased from -0.8730 eV in MoSe₂/HfSe₂/mica to -0.8755 eV in MoSe₂/HfSe₂/MoSe₂/mica, while LUMO state has increased from 0.8450 eV to 0.9773 eV (LUMO (1)) and 0.9820 eV (LUMO (2)) (there are two LUMO states for MoSe₂/HfSe₂/MoSe₂/mica structure) by adding another ML of MoSe₂ between HfSe₂ and mica.

To evaluate how is the charge flow in both interfaces, the HOMO-LUMO isosurfaces have been simulated in Fig. 4, show the charge density redistribution in MoSe₂/HfSe₂/mica and MoSe₂/HfSe₂/MoSe₂/mica systems. In the HOMO state of MoSe₂/HfSe₂/mica, the charge density has delocalized in the molecular orbitals of the substrate (K, O and Al atoms) and MoSe₂ layer, then in the LUMO state, a major part of the charges has accumulated on the HfSe₂ layer. About the charge

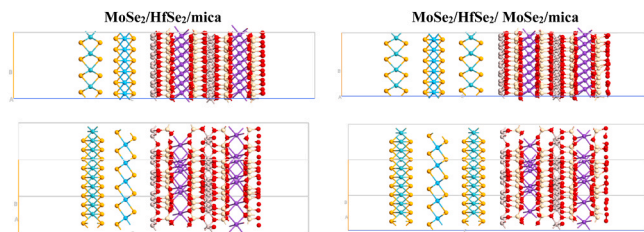


Fig. 3. The modeled structures of the MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂ vdW heterostructure on mica by different views; the dark-blue, gold, and light-blue sticks are the Mo, Se, and Hf atoms, respectively. The mica atoms coloured in O (red), Si (yellow), Al (brown), P (violet), and H (white).

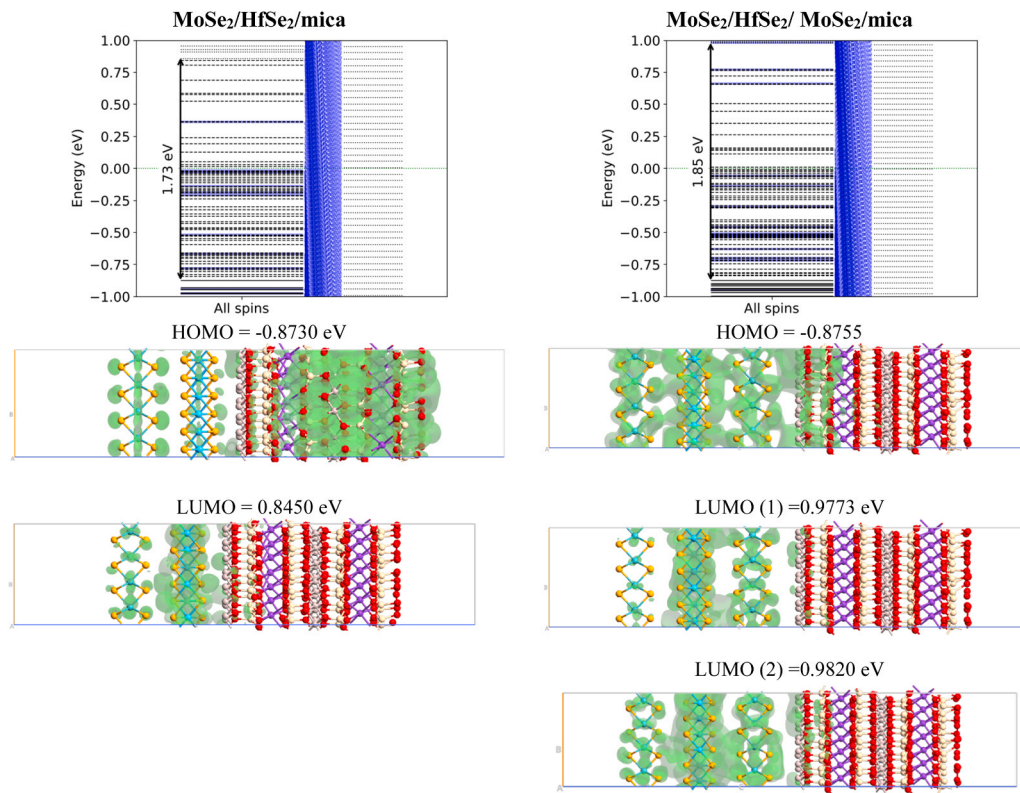


Fig. 4. MES calculations including the HOMO-LUMO band gaps and split energies as well as isosurfaces of HOMO and LUMO states of $\text{MoSe}_2/\text{HfSe}_2/\text{mica}$ and $\text{MoSe}_2/\text{HfSe}_2/\text{MoSe}_2/\text{mica}$ interfaces. The dark-blue, gold, and light-blue sticks are the Mo, Se, and Hf atoms, respectively. The mica atoms coloured in O (red), Si (yellow), Al (brown), and P (violet), with H (white).

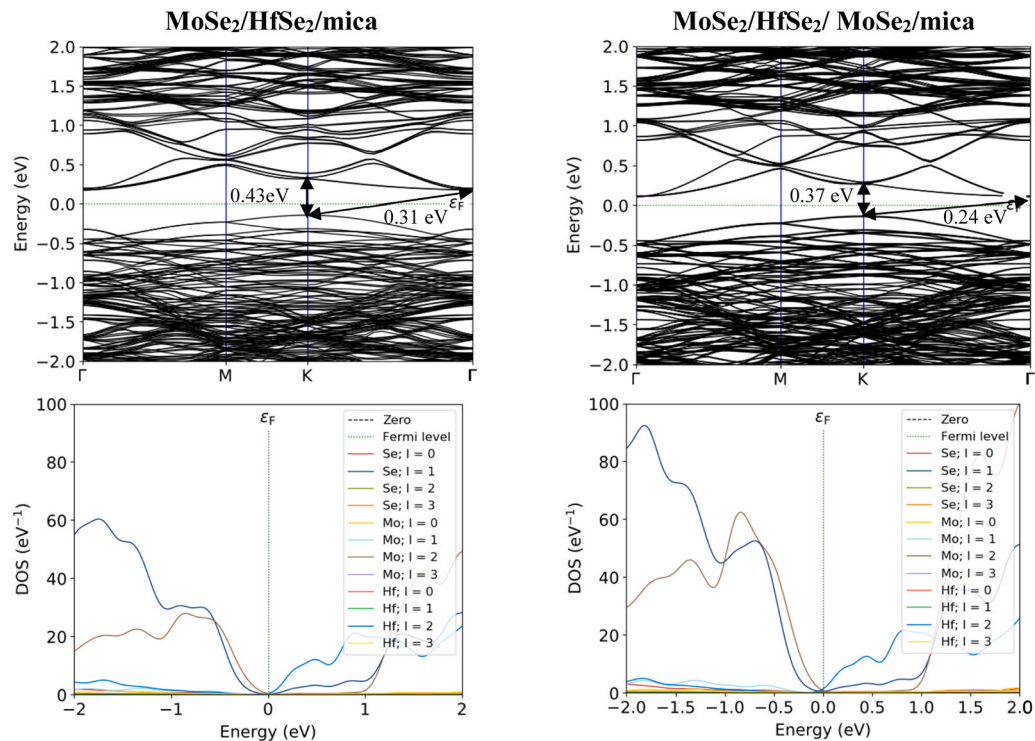
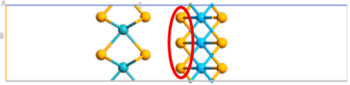
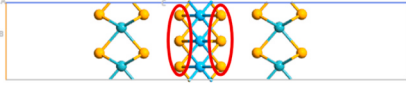


Fig. 5. The corresponding band structure and PDOS plots including SOC calculations of $\text{MoSe}_2/\text{HfSe}_2$ and $\text{MoSe}_2/\text{HfSe}_2/\text{MoSe}_2$ heterostructures on mica substrate along the high-symmetry directions in their first Bz. In the PDOS calculations curves the atomic shells of s, p, d and f labeled in l = 0,1,2, and 3.

Table 1Mulliken charge calculations of HfSe₂, MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂ including total and different shells.

HfSe ₂	Total Shell	Total Shell
	Hf 11.692 2.775 (s)	Se 16.154 1.887 (s)
	6.005 (p)	4.265 (p)
	2.707 (d)	10.00 (d)
	0.206 (f)	0.002 (f)
	Total Shell	Total Shell
	Hf 11.603 2.763 (s)	Se 16.282 1.892 (s)
	6.006 (p)	4.387 (p)
	2.638 (d)	10.00 (d)
	0.196 (f)	0.002 (f)
	Total Shell	Total Shell
	Hf 11.551 2.747 (s)	Se 16.253 1.970 (s)
	6.007 (p)	4.359 (p)
	2.606 (d)	10.00 (d)
	0.192 (f)	0.002 (f)

delocalization in MoSe₂/HfSe₂/MoSe₂/mica system, whereas in the HOMO state the charges have redistributed on the TMDs layers and a bit on mica, the LUMO state has occupied mostly on the HfSe₂ layer similar to what we have seen in MoSe₂/HfSe₂/mica vdW heterostructure. With a comparison of the charge flow and structural parameters of these heterostructures, the outcomes shown that the reason why the mica-HfSe₂ interlayer distance in MoSe₂/HfSe₂/mica is lower than that of mica-MoSe₂ in MoSe₂/HfSe₂/MoSe₂/mica, while the TMDs layer distance of MoSe₂-HfSe₂ has revealed shorter value of distance in MoSe₂/HfSe₂/MoSe₂/mica.

According to the studies based on TMDs monolayers (such as MoS₂ or WS₂) exfoliated onto muscovite mica, the charge flow is from the mica to the TMD layer. Mica is known to act as an electron donor, introducing *n*-type doping into 2D materials placed on its surface due to charge transfer from trap states [83,84]. However, the primary charge flow occurs between the semiconductor layers rather than from the mica substrate. The mica primarily serves as a mechanical support and dielectric environment rather than an active participant in charge flow.

After considering the structural parameters and charge flow properties of the vdW heterostructures, we cut the mica substrate from the modelled supercells, and we reinvestigated their properties to compare them with the MLs systems. Based on the SOGGA calculations for MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂ band properties (Fig. 5), the predicted direct/indirect band gaps have estimated to be 0.43 eV/0.31 eV and 0.37 eV/0.24 eV from K→K/Γ→K, respectively. PDOS calculations have revealed a band attributed to Hf 5d orbitals (Hf = I(2)) immediately above the Fermi energy (*E_F*), while below the *E_F* there are bands related to the Mo 5d (Mo = I(2))) and Se 4p (Se = I(1))) contributions. From our DFT calculations, we have concluded that the CBE of MoSe₂/HfSe₂/MoSe₂ is located at the M-point in the Brillouin zone, which is contributed by the HfSe₂ monolayer, while the VBE is positioned at the K-point, contributed by the MoSe₂, leading to a type II band alignment similar to the one observed in the WSe₂/MoS₂ system [85]. Type II band alignment is important in photodetection and carrier transport [86].

Next, we examined the amount of charge transfer between the atoms and the layers with Mulliken charge calculations. The results showed that, the electron accumulation takes place in the HfSe₂ layer in both heterostructures and MoSe₂ nanosheets lost the electron. This is another reason for type- II semiconductor of MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂ in which VBE loses electrons and CBE gains electrons. As an important factor when adjusting the field-emission features of electronic devices, the work function *W_F* describes the energy difference between the vacuum and Fermi levels. Since the electrons are transferred from the material with smaller *W_F* to that with larger *W_F*, in the both vdW heterostructure, the charges will be transferred from the MoSe₂ (4.30) layer to the HfSe₂ (5.30) layer [29]. On the other hand, while Se atoms with higher electronegativity (2.55) in HfSe₂ ML do receive charge from Hf with lower electronegativity (1.33), leading to an charge

redistribution, the Mo atoms possess electronegativity (2.16) lower than Se atoms in MoSe₂, then the difference in electronegativity between the metal and the chalcogen atoms drives less charge transfer.

Since the main accumulation of the charges are in the middle of interfaces, we collected the data related to total and different shells of HfSe₂ layer in pristine and interfaced structures of MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂. According to Table 1, the charge depletion can be seen for Hf atoms, while charge accumulation corresponds to Se atoms. The quantitatively analysing indicate that the average loss of each Hf atom for the newly proposed model of MoSe₂/HfSe₂ for total charge is 0.089 including *s* (0.01), *d* (0.069) and *f* (0.01) orbitals respect to the same shells in the isolated HfSe₂. These values are becoming more lower in MoSe₂/HfSe₂/MoSe₂ heterostructure with 0.141 in comparison to the pristine HfSe₂. The average gain of each Se atom is 0.128 and 0.099 by the *s* and *p* shells in MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂, respectively. More intriguingly, we found that six Se atoms (connected to Hf atoms) in the MoSe₂/HfSe₂/MoSe₂ are all participated in charge transfer, while in MoSe₂/HfSe₂ more those situated in the side of MoSe₂ received the charges (red shapes in the Table 1, shows the Se atoms participated in the charge transfer for each interface). Therefore, we can conclude that MoSe₂ can influence the Hf and Se atoms for more charge transfer between them. The redistribution of charge in the center of the MoSe₂/HfSe₂/MoSe₂ interface will prevent the recombination of charge carriers, which can significantly change the optical and transport performance of the interface. Also, as we expected, the results showed that there is no interlayer interaction between vdW layers and the electronic structure of heterostructures simply had the superposition of the electronic structures of the MLs.

Then, we evaluated the transport properties of the MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂ heterostructures by considering the mobility, carrier density, and thermal conductivity parameters (Table 2). According to the DFT results, at the temperature of 300° K, for MoSe₂/HfSe₂, a mobility of 0.16 cm² V⁻¹s⁻¹ (with carrier density = 2.24 × 10¹⁵ cm⁻³) contributed to linear response tensors of 0.09 cm²V⁻¹s⁻¹ and 0.073 cm²

Table 2Mobility, carrier density, and thermal conductivity parameters of the MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂ heterostructures.

Interfaces	Mobility (cm ² V ⁻¹ s ⁻¹)	Carrier density (cm ⁻³)	Thermal conductivity (JS ⁻¹ m ⁻¹ K ⁻¹)
MoSe ₂ /HfSe ₂	Total = 0.16	2.24 × 10 ¹⁵	Total = 0.00014
	In-plane (xx) = 0.09		In-plane (xx) = 0.000815
	In-plane (yy) = 0.073		In-plane (yy) = 0.000635
MoSe ₂ /HfSe ₂ /MoSe ₂	Total = 52.1	2.91 × 10 ¹²	Total = 0.58
	In-plane (xx) = 16.6		In-plane (xx) = 0.187
	In-plane (yy) = 35.5		In-plane (yy) = 0.401

$V^{-1}s^{-1}$ along the xx - and yy -in-plane directions, respectively. A corresponding mobility at the same temperature yielded a relatively higher mobility value of $52.1 \text{ cm}^2 V^{-1}s^{-1}$ and a lower carrier density of $2.91 \times 10^{12} \text{ cm}^{-3}$ for the $\text{MoSe}_2/\text{HfSe}_2/\text{MoSe}_2$ heterostructure, with relevant tensor values of $16.6 \text{ cm}^2 V^{-1}s^{-1}$ and $35.5 \text{ cm}^2 V^{-1}s^{-1}$ along the xx - and yy -in-plane directions, respectively.

Due to the quantum confinement effect, the band offsets significantly influence the excited carrier's redistribution [29,87]. The enhanced mobility and improved charge transport in $\text{MoSe}_2/\text{HfSe}_2/\text{MoSe}_2$ rather than $\text{MoSe}_2/\text{HfSe}_2$ stem from several key physical phenomena. The evaluation of the band gap of the interfaces indicates that the lower electronic indirect band gap of $\text{MoSe}_2/\text{HfSe}_2/\text{MoSe}_2$ (0.24 eV), resulted from the more charge redistribution between the atoms as a consequence of lower interlayer distances between TMDs layers. Moreover, experimental studies have highlighted the symmetrical arrangement of HfSe_2 monolayer between two MoSe_2 layers creates highly ordered interface, reducing the interfacial defects and atomic mismatch that traditionally acts as scattering centres and degrades mobility [88,89]. On the other hand, the top and bottom MoSe_2 layers in $\text{MoSe}_2/\text{HfSe}_2/\text{MoSe}_2$ provide a highly effective dielectric environment. This symmetrical dielectric encapsulation heavily screens coulomb impurities (such as trapped charges), a benefit that is asymmetric and less effective when HfSe_2 is exposed to a mica substrate on one side [90]. More, in pristine HfSe_2 , charge transport is limited by optical phonon scattering. Encasing the channel in symmetrical MoSe_2 modifies the local dielectric and vibrational properties, suppressing intervalley and optical-phonon scattering [14].

Moreover, the calculated data obtained from the thermal conductivity in Table 2 indicate ultralow values of $0.00014 \text{ Js}^{-1}\text{m}^{-1}\text{K}^{-1}$ (in-plane xx) = $0.000815 \text{ Js}^{-1}\text{m}^{-1}\text{K}^{-1}$ and in-plane yy) = $0.000635 \text{ Js}^{-1}\text{m}^{-1}\text{K}^{-1}$ for $\text{MoSe}_2/\text{HfSe}_2$, and slightly higher values of $0.58 \text{ Js}^{-1}\text{m}^{-1}\text{K}^{-1}$ (in-plane xx) = $0.187 \text{ Js}^{-1}\text{m}^{-1}\text{K}^{-1}$ and in-plane yy) = $0.401 \text{ Js}^{-1}\text{m}^{-1}\text{K}^{-1}$ for the $\text{MoSe}_2/\text{HfSe}_2/\text{MoSe}_2$ heterostructure, respectively. It should be noted that the lattice thermal conductivity of

the HfSe_2 monolayer calculated by Xiang et al. [91] was predicted to be $5.54 \text{ Wm}^{-1}\text{K}^{-1}$ ($0.00554 \text{ Js}^{-1}\text{m}^{-1}\text{K}^{-1}$) (owing to the stronger phonon scattering and lower velocity of the phonon group), while an even lower value of $1.23 \text{ Wm}^{-1}\text{K}^{-1}$ ($0.00123 \text{ Js}^{-1}\text{m}^{-1}\text{K}^{-1}$) was by Mohanta et al. [92]. On the other hand, the calculated thermal conductivities extracted from atomistic simulations also showed a value of $17.6 \text{ Wm}^{-1}\text{K}^{-1}$ ($0.0176 \text{ Js}^{-1}\text{m}^{-1}\text{K}^{-1}$) for monolayer MoSe_2 [93]. These DFT-based data have confirmed the weak effect of MoSe_2 thickness on the thermal conductivity, i.e., when increasing the number of sample layers, the thermal conductivities do not change remarkably. Furthermore, if any other effect is produced, it should be the opposite for graphite, which shows an increase in thermal conductivity upon decreasing crystal thickness, with monolayered graphene exhibiting the highest thermal conductivity [93,94]. This fact can be supported by our findings related to $\text{MoSe}_2/\text{HfSe}_2$ and $\text{MoSe}_2/\text{HfSe}_2/\text{MoSe}_2$ heterostructures, wherein increasing the MoSe_2 layer slightly improved the thermal conductivity parameter. Furthermore, the reason for the drop in the thermal properties of the vdW heterostructures may be due to the relaxation of hot electrons forming unoccupied states. This leads to a high density of hot electrons dispersing over unoccupied states, which reduces their sensitivity to temperature; in other words, thermal drop prolongs electron-hole pairing [95].

Based on Fig. 6 and the range of photon energy (THz) used, the $\text{MoSe}_2/\text{HfSe}_2$ and $\text{MoSe}_2/\text{HfSe}_2/\text{MoSe}_2$ heterostructures yielded an intensity of absorption first peaks in the region of ~ 0 –9000 cm^{-1} . It's important to remark that the calculated peaks correspond specifically to infrared-active phonon modes (such as transverse and longitudinal optical phonons or acoustic branches) rather than electronic transitions. The DFT data show that the presence of the first peaks at 36 THz with the intensity of 8207 cm^{-1} (xx - in-plane) and 6819 cm^{-1} (yy - in-plane), while along the out-of-plane direction the peak is positioned at 145 THz with intensity of 1750 cm^{-1} . Indeed, one more peak at lower THz frequency is present in the optical absorption spectrum of $\text{MoSe}_2/\text{HfSe}_2/\text{MoSe}_2$ interface at 12.08 THz with the intensity of 3441 cm^{-1} (along the

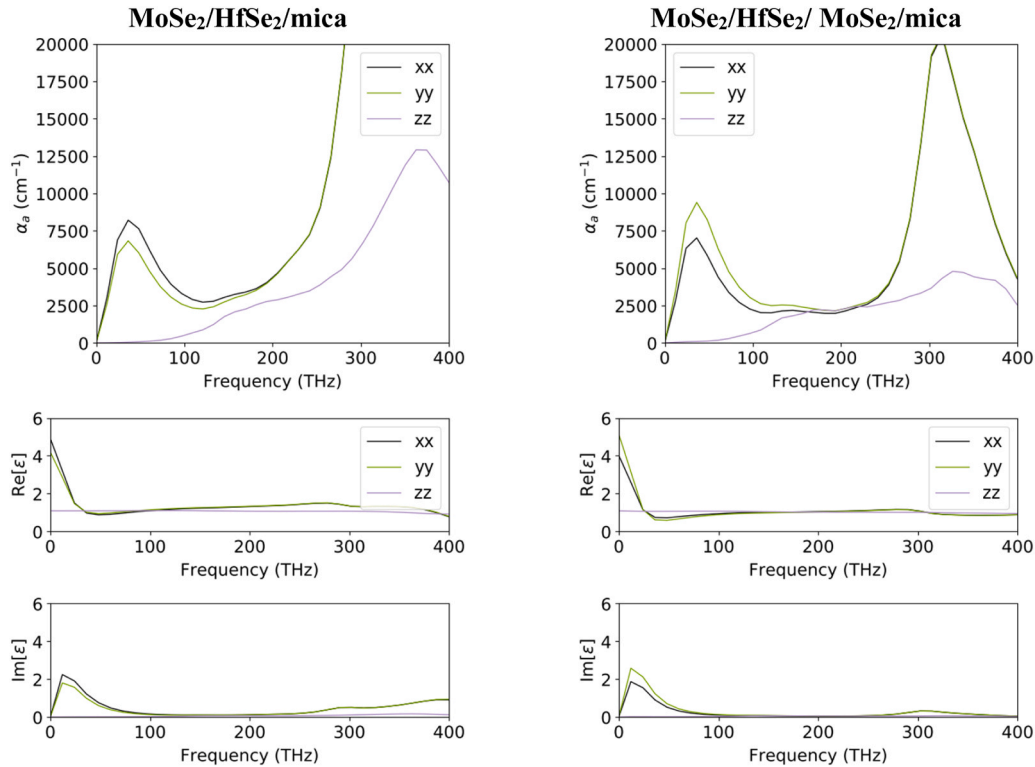


Fig. 6. The optical adsorption and imaginary and real part of dielectric constants of the $\text{MoSe}_2/\text{HfSe}_2$ and $\text{MoSe}_2/\text{HfSe}_2/\text{MoSe}_2$ heterostructures on mica substrate, up to 400 THz frequency range.

in-plane (yy)), and two other peaks at 36.26 THz and 120 THz with relevant intensities of 9393 cm^{-1} and 1263 cm^{-1} along the in-plane(xx) and out-of-plane(zz) directions, respectively. These results indicate that adding another layer of MoSe₂ in MoSe₂/HfSe₂/MoSe₂ heterostructure is a precise method to modify the adsorption intensity along the in-plane and/or out-of-plane directions by altering the interlayer coupling and the electronic structure of the materials.

Notably, the optical structures of MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂ provided significant improvements than MoSe₂ and HfSe₂ MLs. While this study focusses on lower THz frequencies (1–5 THz) for interlayer modes, the peaks around 12 THz and 36 THz ranges in vdW interfaces represent higher-frequency collective vibrations or potential phononic band gap boundaries in stacked layers. 12 THz Region often corresponds to intermediate-frequency interlayer phonons. In multi-layer structures, these modes are attributed to the weak vdW coupling between the chalcogen atoms of adjacent layers. On the other hand, 36 THz region typically corresponds to higher-frequency, intra-layer phonon modes (optical phonons) [96].

Moreover, for the interface of MoSe₂/HfSe₂, the $\text{Re}(\omega)$ are 4.91 and 1.09 along the in-plane(xx) and out-of-plane(zz) polarization directions, while those related to MoSe₂/HfSe₂/MoSe₂ showed higher values at 7.84 and 2.85 along in-plane(yy) and out-of-plane(zz) polarization directions, respectively. More, the $\text{Im}(\omega)$ of the dielectric constant of both interfaces indicated two small peaks in the range of 0–45 THz (could be assigned to intraband transition when compared with the zero values yielded by the MoSe₂ and HfSe₂ nanosheets) along the in-plane direction but different axis similar to what we have for adsorption optical properties.

4. Conclusions

In this work, the electronic, charge transfer, transport and optical properties of MoSe₂ and HfSe₂ nanosheets have compared to MoSe₂/HfSe₂/mica and MoSe₂/HfSe₂/MoSe₂/mica vdW interfaces through first-principles calculations including SOC field. After full optimization of the heterostructure lattices, the HOMO-LUMO band gap and their isosurfaces have been modelled for vdW interface systems. While in both interfaces the LUMO states showed that the charge density accumulation on the molecular orbitals of HfSe₂ ML, the HOMO state highlighted the charge delocalization on the mica and MoSe₂ monolayer in MoSe₂/HfSe₂/mica heterostructure rather than the primary responsibility of the TMDs layers for charge redistribution in MoSe₂/HfSe₂/MoSe₂/mica. Based on the DFT results, the predicted band gaps of MoSe₂, HfSe₂, MoSe₂/HfSe₂ and MoSe₂/HfSe₂/MoSe₂ have direct/indirect band gaps of 1.44 eV(K→K), 1.20 eV(Γ→M), 0.43 eV /0.31 eV and 0.37 eV/0.24 eV both from K→K/Γ→K, respectively. The Mulliken charge calculations indicated that HfSe₂ constitutes the center of electron accumulation in the heterostructure, and the influence of interlayer coupling can only modulate the values of the band gap via the superposition of monolayered electronic structures. An electron mobility of $52.1\text{ cm}^2\text{ V}^{-1}\text{ s}^{-1}$ was calculated, with a carrier density of $2.91 \times 10^{12}\text{ cm}^{-3}$ for the MoSe₂/HfSe₂/MoSe₂ vdW heterostructure, and a very low lattice thermal conductivity of $0.58\text{ Js}^{-1}\text{ m}^{-1}\text{ K}^{-1}$ was predicted for this interface. While the optical adsorption property of MoSe₂/HfSe₂ showed the presence of the first peaks at 36 THz and 145 THz along the in-plane and out-of-plane directions, respectively, the optical absorption spectrum in MoSe₂/HfSe₂/MoSe₂ interface has resulted another peak at lower THz frequency of 12.08 THz, leading to remarkable improvement to the optical properties of the nanosheet systems. The DFT simulation revealed how the presence of the second layer of MoSe₂ in MoSe₂/HfSe₂/MoSe₂ can change the static dielectric constant along the different in-plane directions as well as interlayer coupling by increasing the value from 4.91 (xx- in-plane) and 1.09 (zz- out-of-plane) in MoSe₂/HfSe₂ to 7.84 and 2.85 along in-plane(yy) and out-of-plane(zz) polarization directions, respectively. According to the theoretical outcomes obtained, constructing vdW heterostructures of MoSe₂ and HfSe₂ MLs

open a way as an efficient strategy for enhancing the performances of 2D materials in future THz applications.

CRedit authorship contribution statement

Eleonora Pavoni: Writing – review & editing, Validation, Project administration. **Pierluigi Stipa:** Writing – review & editing, Validation, Supervision, Project administration, Conceptualization. **Elaheh Mohebbi:** Writing – review & editing, Writing – original draft, Visualization, Validation, Project administration, Methodology, Investigation, Data curation, Conceptualization. **Emiliano Laudadio:** Writing – review & editing, Validation, Project administration, Methodology, Conceptualization. **Davide Mencarelli:** Writing – review & editing, Validation, Project administration. **Marina Petroselli:** Writing – review & editing, Validation, Data curation. **Luca Pierantoni:** Writing – review & editing, Validation, Project administration.

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

References

- [1] M. Chhowalla, H.S. Shin, G. Eda, L.-J. Li, K.P. Loh, H. Zhang, The chemistry of two-dimensional layered transition metal dichalcogenide nanosheets, *Nat. Chem.* 5 (2013) 263–275.
- [2] R. Lv, J.A. Robinson, R.E. Schaak, D. Sun, Y. Sun, T.E. Mallouk, M. Terrones, Transition metal dichalcogenides and beyond: synthesis, properties, and applications of single and few-layer nanosheets, *Acc. Chem. Res.* 48 (2015) 56–64.
- [3] M. Ali, A.M. Afzal, M.W. Iqbal, S. Mumtaz, M. Imran, F. Ashraf, A. Ur Rehman, F. Muhammad, 2D-TMDs based electrode material for supercapacitor applications, *Int. J. Energy Res.* 46 (2022) 22336–22364.
- [4] H.R. Gutiérrez, N. Perea-López, A.L. Elías, A. Berkdemir, B. Wang, R. Lv, F. López-Urías, V.H. Crespi, H. Terrones, M. Terrones, Extraordinary room-temperature photoluminescence in triangular WS₂ monolayers, *Nano Lett.* 13 (2013) 3447–3454.
- [5] K.F. Mak, K. He, J. Shan, T.F. Heinz, Control of valley polarization in monolayer MoS₂ by optical helicity, *Nat. Nanotechnol.* 7 (2012) 494–498.
- [6] M. Kumar, S. Rani, P. Vashishtha, G. Gupta, X. Wang, V.N. Singh, Exploring the optoelectronic properties of SnSe: a new insight, *J. Mater. Chem. C. Mater.* 10 (2022) 16714–16722.
- [7] Y. Jeong, H.J. Lee, J. Park, S. Lee, H.-J. Jin, S. Park, H. Cho, S. Hong, T. Kim, K. Kim, Engineering MoSe₂/MoS₂ heterojunction traps in 2D transistors for multilevel memory, multiscale display, and synaptic functions, *NPJ 2D Mater. Appl.* 6 (2022) 23.
- [8] S. Larentis, B. Fallahazad, E. Tutuc, Field-effect transistors and intrinsic mobility in ultra-thin MoS₂ layers, *Appl. Phys. Lett.* 101 (2012).
- [9] B. Chamlagain, Q. Li, N.J. Ghimire, H.J. Chuang, M.M. Perera, H. Tu, Y. Xu, M. Pan, D. Xiao, J. Yan, D. Mandrus, Z. Zhou, Mobility improvement and temperature dependence in MoSe₂ field-effect transistors on parylene-C substrate, *ACS Nano* 8 (2014) 5079–5088, <https://doi.org/10.1021/nn501150r>.
- [10] W. Zhang, Z. Huang, W. Zhang, Y. Li, Two-dimensional semiconductors with possible high room temperature mobility, *Nano Res.* 7 (2014) 1731–1737.
- [11] T. Matić, T. Švedek, M. Hecceg, Comparison of current-voltage characteristics for hypothetical Si and SiC bipolar junction transistor, *Elektro ški Vestn.* 75 (2008) 97–104.
- [12] C.N. Ahmad, A.R. Adams, G.D. Pitt, Temperature dependence of the electron mobility in the $\Delta 1c$ minima of Germanium, *J. Phys. C Solid. State Phys.* 12 (1979) L379.
- [13] C. Gaiser, T. Zandt, A. Krapf, R. Serverin, C. Janowitz, R. Manzke, Band-gap engineering with HfS_x Se_{2-x}, *Phys. Rev. B* 69 (2004) 075205.

- [14] S.P. Keshri, S.K. Pati, A. Medhi, HfSe₂: Unraveling the microscopic reason for experimental low mobility, *J. Chem. Phys.* 159 (2023).
- [15] J.O. Island, A. Kuc, E.H. Diependaal, R. Bratschkitsch, H.S.J. Van Der Zant, T. Heine, A. Castellanos-Gomez, Precise and reversible band gap tuning in single-layer MoSe₂ by uniaxial strain, *Nanoscale* 8 (2016) 2589–2593.
- [16] Z. Lin, H. Yan, J. Liu, Y. An, Defects engineering monolayer MoSe₂ magnetic states for 2D spintronic device, *J. Alloy. Compd.* 774 (2019) 160–167.
- [17] S. Tongay, J. Zhou, C. Ataca, K. Lo, T.S. Matthews, J. Li, J.C. Grossman, J. Wu, Thermally driven crossover from indirect toward direct bandgap in 2D semiconductors: MoSe₂ versus MoS₂, *Nano Lett.* 12 (2012) 5576–5580.
- [18] Q. Yao, L. Zhang, P. Bampoulis, H.J.W. Zandvliet, Nanoscale investigation of defects and oxidation of HfSe₂, *J. Phys. Chem. C* 122 (2018) 25498–25505.
- [19] H. Habib, W. Zhao, S. Mir, L. Ma, G. Tian, Strongly enhanced infrared absorption of HfSe₂ monolayer by lanthanide doping: A first-principles study, *Results Phys.* 48 (2023) 106415.
- [20] H.Y. Lv, W.J. Lu, X. Luo, H.Y. Lu, X.B. Zhu, Y.P. Sun, Enhancing the thermoelectric performance of a HfS₂ monolayer through valley engineering, *ArXiv Preprint ArXiv:1608.05464* (2016).
- [21] R. Cheng, D. Li, H. Zhou, C. Wang, A. Yin, S. Jiang, Y. Liu, Y. Chen, Y. Huang, X. Duan, Electroluminescence and photocurrent generation from atomically sharp WSe₂/MoS₂ heterojunction p–n diodes, *Nano Lett.* 14 (2014) 5590–5597.
- [22] T. Yang, B. Zheng, Z. Wang, T. Cui, C. Pan, J. Zou, X. Zhang, Z. Qi, H. Liu, Y. Feng, Van der Waals epitaxial growth and optoelectronics of large-scale WSe₂/SnS₂ vertical bilayer p–n junctions, *Nat. Commun.* 8 (2017) 1906.
- [23] J. Xia, J. Yan, Z. Wang, Y. He, Y. Gong, W. Chen, T.C. Sum, Z. Liu, P.M. Ajayan, Z. Shen, Strong coupling and pressure engineering in WSe₂–MoSe₂ heterobilayers, *Nat. Phys.* 17 (2021) 92–98.
- [24] E. Mohebbi, E. Pavoni, L. Pierantoni, P. Stipa, G.M. Zampa, E. Laudadio, D. Mencarelli, Band gap and THz optical adsorption of SnSe and SnSe₂ nanosheets on graphene: Negative dielectric constant of SnSe, *Results Phys.* (2024) 107415.
- [25] E. Mohebbi, E. Pavoni, P. Stipa, L. Pierantoni, E. Laudadio, D. Mencarelli, Tunable Optical Properties of Cu/VSe₂ from the Visible to Terahertz Spectral Range: A First-Principles Study, *Int. J. Mol. Sci.* 26 (2025) 2527.
- [26] K.E. Aretouli, P. Tsipras, D. Tsoutsou, J. Marquez-Velasco, E. Xenogiannopoulou, S. A. Giamini, E. Vassalou, N. Kelaidis, A. Dimoulas, Two-dimensional semiconductor HfSe₂ and MoSe₂/HfSe₂ van der Waals heterostructures by molecular beam epitaxy, *Appl. Phys. Lett.* 106 (2015).
- [27] Y. Wang, X. Jing, L. Bai, D. Pan, W. Wang, F. Lu, X. Fu, X. Liu, X. Ding, J. Deng, Preparation and optoelectronic performance of two-dimensional MoSe₂/WSe₂ lateral and vertical heterostructures, *Mater. Today Phys.* 43 (2024) 101404.
- [28] M.O. Li, D. Esseni, G. Snider, D. Jena, H. Grace Xing, Single particle transport in two-dimensional heterojunction interlayer tunneling field effect transistor, *J. Appl. Phys.* 115 (2014).
- [29] W. Ju, Y. Zhang, T. Li, D. Wang, E. Zhao, G. Hu, Y. Xu, H. Li, A type-II WSe₂/HfSe₂ van der Waals heterostructure with adjustable electronic and optical properties, *Results Phys.* 25 (2021) 104250.
- [30] A. Li, Z. Yang, Z. Long, F. Huang, Z. Chen, Design and performance evaluation of flexible terahertz ultra-wideband stop-band filters, *Appl. Opt.* 64 (2025) 2028–2036.
- [31] O. Tervo, T. Levanen, K. Pajukoski, J. Hultkonen, P. Wainio, M. Valkama, 5G new radio evolution towards sub-THz communications. 2020 2nd 6G Wireless Summit (6G Summit), *IEEE*, 2020, pp. 1–6.
- [32] Y. Zhang, C. Wang, B. Huai, S. Wang, Y. Zhang, D. Wang, L. Rong, Y. Zheng, Continuous-wave THz imaging for biomedical samples, *Appl. Sci.* 11 (2020) 71.
- [33] S. Sharma, P.K. Singya, K. Deka, C. Adijh, M. Sharma, Terahertz communication: State-of-the-art and future directions, *IEEE Open. J. Commun. Soc.* (2025).
- [34] X. Li, J. Li, Y. Li, A. Ozcan, M. Jarrahi, High-throughput terahertz imaging: progress and challenges, *Light. Sci. Appl.* 12 (2023) 233.
- [35] E. Mohebbi, E. Pavoni, L. Pierantoni, P. Stipa, E. Laudadio, D. Mencarelli, Effect of different pseudopotentials on the phonon frequencies, dielectric constant, and Born effective charge of SnSe and SnSe₂ nanostructures: A density functional perturbation theory study, *J. Phys. Chem. Solids* 185 (2024) 111755.
- [36] E. Pavoni, E. Mohebbi, G.M. Zampa, P. Stipa, L. Pierantoni, E. Laudadio, D. Mencarelli, First principles study of WSe₂ and the effect of V doping on the optical and electronic properties, *Mater. Adv.* (2024).
- [37] E. Mohebbi, E. Pavoni, P. Stipa, M. Petroselli, C. Minnelli, L. Pierantoni, D. Mencarelli, M. Aldrigo, E. Laudadio, M.M.S. Fakhraabadi, Electronic structure of 1, 4-Phenylenediacrylic acid on graphene and bilayer graphite: from experiments to DFT and ab initio molecular dynamics simulations, *Chem. Phys. Impact* (2025) 100947.
- [38] E. Mohebbi, E. Pavoni, P. Stipa, M. Petroselli, L. Pierantoni, E. Laudadio, D. Mencarelli, Reliable prediction of the band gap properties of graphene buffer layer on SiC using meta-GGA approximation, *Carbon Trends* (2025) 100575.
- [39] M.T. Dau, C. Vergnaud, M. Gay, C.J. Alvarez, A. Marty, C. Beigné, D. Jalabert, J.-F. Jacquot, O. Renault, H. Okuno, van der Waals epitaxy of Mn-doped MoSe₂ on mica, *APL Mater.* 7 (2019).
- [40] X. Zou, J. Xu, L. Liu, H. Wang, P.-T. Lai, W.M. Tang, Damage-free mica/MoSe₂ interface for high-performance multilayer MoS₂ field-effect transistors, *Nanotechnology* 30 (2019) 345204.
- [41] S. Li, D. Ouyang, N. Zhang, Y. Zhang, A. Murthy, Y. Li, S. Liu, T. Zhai, Substrate engineering for chemical vapor deposition growth of large-scale 2D transition metal dichalcogenides, *Adv. Mater.* 35 (2023) 2211855.
- [42] Y. Wang, X. Jing, L. Bai, D. Pan, W. Wang, F. Lu, X. Fu, X. Liu, X. Ding, J. Deng, Preparation and optoelectronic performance of two-dimensional MoSe₂/WSe₂ lateral and vertical heterostructures, *Mater. Today Phys.* 43 (2024) 101404.
- [43] S. Smidstrup, T. Markussen, P. Vancraeyveld, J. Wellendorff, J. Schneider, T. Gunst, B. Verstichel, D. Stradi, P.A. Khomyakov, U.G. Vej-Hansen, QuantumATK: An integrated platform of electronic and atomic-scale modelling tools, *J. Phys. Condens. Matter* 32 (2019) 015901.
- [44] E. Pavoni, E. Mohebbi, P. Stipa, L. Pierantoni, D. Mencarelli, M. Dragoman, M. Aldrigo, E. Laudadio, First-principles investigation of interface phenomena in hafnium-based metal–insulator–metal diodes, *Nanoscale Adv.* 5 (2023) 2748–2755.
- [45] E. Laudadio, E. Mohebbi, E. Pavoni, C. Minnelli, S. Sabbatini, P. Stipa, Density functional theory and molecular dynamics studies on electrical, mechanical, and thermal properties of TiO₂ nanoparticles interacting with poly lactic-co-glycolic acid, *Colloids Surf. A Physicochem. Eng. Asp.* 667 (2023) 131388.
- [46] E. Mohebbi, E. Pavoni, L. Pierantoni, P. Stipa, E. Laudadio, D. Mencarelli, Insights Into a New Geometric Graphene Diode with Ultrahigh Asymmetry Ratio: A Computational Approach, in: *IEEE 23rd International Conference on Nanotechnology (NANO)*, 2023, *IEEE*, 2023, pp. 238–242.
- [47] E. Mohebbi, E. Pavoni, L. Pierantoni, P. Stipa, A. Hemmetter, E. Laudadio, D. Mencarelli, Towards graphene-based asymmetric diodes: a density functional tight-binding study, *Nanoscale Adv.* (2024).
- [48] W. Kohn, L.J. Sham, Self-consistent equations including exchange and correlation effects, *Phys. Rev.* 140 (1965) A1133.
- [49] M. Ernzerhof, G.E. Scuseria, Perspective on “Inhomogeneous electron gas” Hohenberg P., Kohn W. (1964) *Phys Rev* 136: B864, *Theor. Chem. Acc.* 103 (2000) 259–262.
- [50] D. Sánchez-Portal, P. Ordejon, E. Artacho, J.M. Soler, Density-functional method for very large systems with LCAO basis sets, *Int. J. Quantum Chem.* 65 (1997) 453–461.
- [51] M.J. van Setten, M. Giantomassi, E. Bousquet, M.J. Verstraete, D.R. Hamann, X. Gonze, G.-M. Rignanese, The PseudoDojo: Training and grading a 85 element optimized norm-conserving pseudopotential table, *Comput. Phys. Commun.* 226 (2018) 39–54.
- [52] Z. Wan, Q. De Wang, D. Liu, J. Liang, Effectively improving the accuracy of PBE functional in calculating the solid band gap via machine learning, *Comput. Mater. Sci.* 198 (2021), <https://doi.org/10.1016/j.commatsci.2021.110699>.
- [53] L. Banu, S. V. Veerapandey, H. Fjellvåg, P. Vajeeston, First-principles insights into the relative stability, physical properties, and chemical properties of MoSe₂, *ACS Omega* 8 (2023) 13799–13812.
- [54] S. Ehrlich, J. Moellmann, W. Reckien, T. Bredow, S. Grimme, System-dependent dispersion coefficients for the DFT-D3 treatment of adsorption processes on ionic surfaces, *ChemPhysChem* 12 (2011) 3414–3420.
- [55] S. Picozzi, Spin–orbit coupling in quantum materials: emergent phenomena, their modelling and examples from two-dimensional magnets, *La Riv. Del. Nuovo Cim.* 47 (2024) 609–652.
- [56] Q. Gu, S.K. Pandey, R. Tiwari, A computational method to estimate spin–orbital interaction strength in solid state systems, *Comput. Mater. Sci.* 221 (2023) 112090.
- [57] M.M.R. Paramanik, First principles calculations of structural, thermophysical, dynamical, electronic and optical properties of the intermetallic compound CoSi, *Results Mater.* (2025) 100743.
- [58] K. Zollner, M. Kurpas, M. Gmitra, J. Fabian, First-principles determination of spin–orbit coupling parameters in two-dimensional materials, *Nat. Rev. Phys.* (2025) 1–15.
- [59] V.O. Özçelik, J.G. Azadani, C. Yang, S.J. Koester, T. Low, Band alignment of two-dimensional semiconductors for designing heterostructures with momentum space matching, *Phys. Rev. B* 94 (2016) 035125.
- [60] Y. Duan, L. Qin, L. Shi, G. Tang, More accurate predictions of band gap tuned by pressure in InN using HSE06 and GW approximations, *Comput. Mater. Sci.* 101 (2015) 56–61.
- [61] K. Zollner, S.M. João, B.K. Nikolić, J. Fabian, Twist-and gate-tunable proximity spin–orbit coupling, spin relaxation anisotropy, and charge-to-spin conversion in heterostructures of graphene and transition metal dichalcogenides, *Phys. Rev. B* 108 (2023) 235166.
- [62] S.-D. Guo, J.-L. Wang, Spin–orbital coupling effect on the power factor in semiconducting transition-metal dichalcogenide monolayers, *Semicond. Sci. Technol.* 31 (2016) 095011.
- [63] M.K. Mohanta, A. De Sarkar, Coupled spin and valley polarization in monolayer HfN₂ and valley-contrasting physics at the HfN₂-WSe₂ interface, *Phys. Rev. B* 102 (2020) 125414.
- [64] D.P. Rai, T.V. Vu, A. Laref, M.A. Hossain, E. Haque, S. Ahmad, R. Khenata, R. K. Thapa, Electronic properties and low lattice thermal conductivity (κ) of monolayer (ML) MoS₂: 2P-LAPW incorporated with spin–orbit coupling (SOC), *RSC Adv.* 10 (2020) 18830–18840.
- [65] D.W. Latzke, W. Zhang, A. Suslu, T.-R. Chang, H. Lin, H.-T. Jeng, S. Tongay, J. Wu, A. Bansil, A. Lanzara, Electronic structure, spin–orbit coupling, and interlayer interaction in bulk MoS₂ and WS₂, *Phys. Rev. B* 91 (2015) 235202.
- [66] T. Gunst, T. Markussen, K. Stokbro, M. Brandbyge, First-principles method for electron-phonon coupling and electron mobility: Applications to 2D materials, *ArXiv Preprint ArXiv:1511.02045* (2015).
- [67] E. Mohebbi, M.M.S. Fakhraabadi, First-principles calculations to investigate strain-tunable electronic bandgap of black phosphorus-structured nitrogen with desirable optical and elastic properties, *Materials Science Engineering B* 281 (2022) 115745.
- [68] J.A. Wilson, A.D. Yoffe, The transition metal dichalcogenides discussion and interpretation of the observed optical, electrical and structural properties, *Adv. Phys.* 18 (1969) 193–335.
- [69] Q.H. Wang, K. Kalantar-Zadeh, A. Kis, J.N. Coleman, M.S. Strano, Electronics and optoelectronics of two-dimensional transition metal dichalcogenides, *Nat. Nanotechnol.* 7 (2012) 699–712.

- [70] X. Wang, Y. Gong, G. Shi, W.L. Chow, K. Keyshar, G. Ye, R. Vajtai, J. Lou, Z. Liu, E. Ringe, Chemical vapor deposition growth of crystalline monolayer MoSe₂, *ACS Nano* 8 (2014) 5125–5131.
- [71] Z. Luo, J. Hao, J. Li, The optical properties of MoSe₂ in bulk and monolayer with different crystal orientation based on first-principles calculations, *Acad. J. Mater. & Chem.* 3 (2022) 51–57.
- [72] S. Li, M. Zhou, X. Wang, F. Zheng, X. Shao, P. Zhang, HfSe₂ monolayer stability tuning by strain and charge doping, *Phys. Lett. A* 384 (2020) 126534.
- [73] J. Xiang, H. Wang, B. Dai, W.-L. Cheng, X.-W. Zhang, Z.-G. Wang, N.-N. Ge, Optimizing the thermoelectric transmission of monolayer HfSe₂ by strain engineering, *J. Phys. Chem. Solids* 169 (2022) 110834.
- [74] B. Scharf, D. Van Tuan, I. Žutić, H. Dery, Dynamical screening of excitons in monolayer transition-metal dichalcogenides, *ArXiv* (1801. 06217 V1) (2018) 1–34.
- [75] N. Alidoust, G. Bian, S.-Y. Xu, R. Sankar, M. Neupane, C. Liu, I. Belopolski, D.-X. Qu, J.D. Denlinger, F.-C. Chou, Observation of monolayer valence band spin-orbit effect and induced quantum well states in MoX₂, *Nat. Commun.* 5 (2014) 1–9.
- [76] B.S. Kim, W.S. Kyung, J.J. Seo, J.Y. Kwon, J.D. Denlinger, C. Kim, S.R. Park, Possible electric field induced indirect to direct band gap transition in MoSe₂, *Sci. Rep.* 7 (2017) 5206.
- [77] M. Rybak, T. Woźniak, M. Birowska, F. Dybala, A. Segura, K.J. Kapcia, P. Scharoch, R. Kudrawiec, Stress-tuned optical transitions in layered 1T-MX₂ (M= Hf, Zr, Sn; X= S, Se) crystals, *Nanomaterials* 12 (2022) 3433.
- [78] E. Xenogiannopoulou, P. Tsipas, K.E. Aretouli, D. Tsoutsou, S.A. Giamini, C. Bazioti, G.P. Dimitrakopoulos, P. Komninou, S. Brems, C. Huyghebaert, High-quality, large-area MoSe₂ and MoSe₂/Bi₂Se₃ heterostructures on AlN (0001)/Si (111) substrates by molecular beam epitaxy, *Nanoscale* 7 (2015) 7896–7905.
- [79] R. Yue, A.T. Barton, H. Zhu, A. Azcatl, L.F. Pena, J. Wang, X. Peng, N. Lu, L. Cheng, R. Addou, HfSe₂ thin films: 2D transition metal dichalcogenides grown by molecular beam epitaxy, *ACS Nano* 9 (2015) 474–480.
- [80] Y.-R. Chang, T. Nishimura, T. Taniguchi, K. Watanabe, K. Nagashio, Performance enhancement of SnS/h-BN heterostructure p-type FET via the thermodynamically predicted surface oxide conversion method, *ACS Appl. Mater. Interfaces* 14 (2022) 19928–19937.
- [81] A. Pezo, S. Massabeau, F. Miljević, J. Li, F. Ibrahim, M. Jamet, M. Chshiev, J.-M. George, H. Jaffrès, Spin and orbital rashba response in ferroelectric polarized PtSe₂/MoSe₂/LiNbO₃ heterostructures, *ArXiv Preprint ArXiv: 2509.16350* (2025).
- [82] H.J. Liu, L. Jiao, L. Xie, F. Yang, J.L. Chen, W.K. Ho, C.L. Gao, J.F. Jia, X.D. Cui, M. H. Xie, Molecular-beam epitaxy of monolayer and bilayer WSe₂: a scanning tunneling microscopy/spectroscopy study and deduction of exciton binding energy, *2d Mater.* 2 (2015) 034004.
- [83] H. Li, S. Kovalchuk, A. Kumar, D. Liang, B.D. Frank, H. Lin, N. Severin, K.I. Bolotin, S. Kirstein, J.P. Rabe, Evidence for charging and discharging of MoS₂ and WS₂ on mica by intercalating molecularly thin liquid layers, *Phys. Status Solidi (a)* 221 (2024) 2300302.
- [84] A. Rauf, J.D. Cojal González, A. Balkan, N. Severin, I.M. Sokolov, J.P. Rabe, Shaping surfaces and interfaces of 2D materials on mica with intercalating water and ethanol, *Mol. Phys.* 119 (2021) e1947534.
- [85] M.-H. Chiu, C. Zhang, H.-W. Shiu, C.-P. Chuu, C.-H. Chen, C.-Y.S. Chang, C.-H. Chen, M.-Y. Chou, C.-K. Shih, L.-J. Li, Determination of band alignment in the single-layer MoS₂/WSe₂ heterojunction, *Nat. Commun.* 6 (2015) 7666.
- [86] Y. Chen, C. Tan, Z. Wang, J. Miao, X. Ge, T. Zhao, K. Liao, H. Ge, Y. Wang, F. Wang, Momentum-matching and band-alignment van der Waals heterostructures for high-efficiency infrared photodetection, *Sci. Adv.* 8 (2022) eabq1781.
- [87] C.G. Van de Walle, J. Neugebauer, Universal alignment of hydrogen levels in semiconductors, insulators and solutions, *Nature* 423 (2003) 626–628.
- [88] D. Tsoutsou, K.E. Aretouli, P. Tsipas, J. Marquez-Velasco, E. Xenogiannopoulou, N. Kelaidis, S. Aminalragia Giamini, A. Dimoulas, Epitaxial 2D MoSe₂ (HfSe₂) semiconductor/2D TaSe₂ metal van der Waals heterostructures, *ACS Appl. Mater. Interfaces* 8 (2016) 1836–1841.
- [89] B. Chamlagain, Q. Li, N.J. Ghimire, H.-J. Chuang, M.M. Perera, H. Tu, Y. Xu, M. Pan, D. Xaio, J. Yan, Mobility improvement and temperature dependence in MoSe₂ field-effect transistors on parylene-C substrate, *ACS Nano* 8 (2014) 5079–5088.
- [90] D. Çakır, F.M. Peeters, Dependence of the electronic and transport properties of metal-MoSe₂ interfaces on contact structures, *Phys. Rev. B* 89 (2014) 245403.
- [91] J. Xiang, H. Wang, B. Dai, W.-L. Cheng, X.-W. Zhang, Z.-G. Wang, N.-N. Ge, Optimizing the thermoelectric transmission of monolayer HfSe₂ by strain engineering, *J. Phys. Chem. Solids* 169 (2022) 110834.
- [92] M.K. Mohanta, A. Rawat, N. Jena, R. Ahammed, A. De Sarkar, Ultra-low lattice thermal conductivity and giant phonon–electric field coupling in hafnium dichalcogenide monolayers, *J. Phys. Condens. Matter* 32 (2020) 315301.
- [93] D. Saleta Reig, S. Varghese, R. Farris, A. Block, J.D. Mehew, O. Hellman, P. Woźniak, M. Sledzinska, A. El Sachat, E. Chávez-Ángel, Unraveling heat transport and dissipation in suspended MoSe₂ from bulk to monolayer, *Adv. Mater.* 34 (2022) 2108352.
- [94] A.A. Balandin, S. Ghosh, W. Bao, I. Calizo, D. Teweldebrhan, F. Miao, C.N. Lau, Superior thermal conductivity of single-layer graphene, *Nano Lett.* 8 (2008) 902–907.
- [95] T.E. Ada, K.N. Nigussa, Van der Waals hetrostructure configuration effect on exciton and thermoelectric characteristics, *ArXiv Preprint ArXiv:2405.10755* (2024).
- [96] P.-J. Wang, P.-C. Tsai, Z.-S. Yang, S.-Y. Lin, C.-K. Sun, Revealing the interlayer van der Waals coupling of bi-layer and tri-layer MoS₂ using terahertz coherent phonon spectroscopy, *Photoacoustics* 28 (2022) 100412.