



A first-principles study of electronic and optical responses of multi-layered PtSe₂ sandwiched between WSe₂ and mica

Elaheh Mohebbi^a, Eleonora Pavoni^a, Pierluigi Stipa^a, Luca Pierantoni^b,
Marina Petroselli^a, Emiliano Laudadio^{a,*}, Davide Mencarelli^b

^a Department of Science and Engineering of Matter, Environment and Urban Planning (SIMAU), Università Politecnica delle Marche, Ancona, 60131, Italy

^b Information Engineering Department, Marche Polytechnic University, Ancona, 60131, Italy

ARTICLE INFO

Keywords:

DFT
van der Waals heterostructures
WSe₂
PtSe₂ multi-layers
THz application

ABSTRACT

An ab initio approach was used to define the structural, electronic, and optical properties of PtSe₂ and WSe₂ as monolayer (ML) systems and four heterostructures based on 1 ML WSe₂ on different thicknesses of PtSe₂, on a mica substrate, as van der Waals (vdW) heterostructures. The MLs of WSe₂ and PtSe₂ exhibited a direct/indirect band gap of 1.68 eV/1.36 eV. In relation to the heterostructures, the increasing PtSe₂ thickness from 1 to 4 MLs affects the interlayer spacing and band alignment, reducing the band gap; moreover, the PtSe₂ thickness increasing brings to a gradual transition from indirect to direct bandgap. PDOS analysis shows that both Pt and W orbitals contributed to the valence band, Pt contribution is dominant in the conduction band, but the Se atoms possess the higher DOS before and after the Fermi level in all the interfaces. The MPSH results indicate an enhanced orbital delocalization, which exhibits the smallest HOMO–LUMO separation. The optical properties in the frequency (THz) range showed that the absorption response depends on the number of layers in the heterostructures, with the WSe₂@3MLPtSe₂ system demonstrating the highest in-plane absorption intensity. However, the real part (Re(ω)) of dielectric function showed the higher values for WSe₂/3MLPtSe₂ with in-plane = 6.54 and out-of-plane = 1.59 than others; this interface indicated higher peak intensity along the in-plane direction in the frequency of 24 THz in the imaginary part (Im(ω)), while WSe₂/1MLPtSe₂ showed the lowest one. These findings demonstrate that WSe₂/3MLPtSe₂ heterostructure exhibited as good candidate for THz optoelectronic applications.

1. Introduction

The terahertz (THz) spectral range, typically defined between 0.1 and 10 THz, has gained increasing attention because of its relevance for imaging, spectroscopy, communication systems, and security technologies [1–3]. The rapid growth of data-intensive applications, including cloud computing, immersive media, and the Internet of Things (IoT), has significantly increased the demand for ultra-high-speed wireless communication systems [1,4,5]. Current wireless networks operating in the microwave and millimeter-wave bands are approaching spectrum congestion, limiting their ability to support future data rate requirements [6,7]. As a result, the exploration of higher carrier frequencies has become a key research direction for next-generation communication technologies [8]. However, the development of efficient THz sources, detectors, and modulators remains challenging due to the

lack of suitable materials exhibiting strong interaction with THz radiation [2,9,10].

Two-dimensional (2D) materials have recently been proposed as promising candidates to overcome these limitations thanks to their tunable electronic properties, ultrafast carrier dynamics, and strong optical interaction [11,12]. Among them, 2D transition metal dichalcogenides (TMDs) have attracted considerable attention in recent years due to their remarkable electronic, optical, and transport properties, which strongly depend on the number of layers and differ significantly from those of their bulk materials. Thanks to their layered nature, these materials exhibit tunable band structures, strong light–matter interaction, and high carrier mobility, making them promising candidates for next-generation electronic and optoelectronic devices [13–16]. TMDs based on tungsten (W) and platinum (Pt) chalcogenides have emerged as versatile platforms for applications ranging from photodetectors to

* Corresponding author

E-mail addresses: e.mohebbi@staff.univpm.it (E. Mohebbi), e.pavoni@staff.univpm.it (E. Pavoni), p.stipa@staff.univpm.it (P. Stipa), l.pierantoni@staff.univpm.it (L. Pierantoni), m.petroselli@pm.univpm.it (M. Petroselli), e.laudadio@staff.univpm.it (E. Laudadio), d.mencarelli@staff.univpm.it (D. Mencarelli).

<https://doi.org/10.1016/j.rsurfi.2026.100938>

Received 9 June 2026; Received in revised form 14 July 2026; Accepted 9 August 2026

Available online 14 August 2026

2666-8459/© 2026 The Authors. Published by Elsevier B.V. This is an open access article under the CC BY-NC-ND license (<http://creativecommons.org/licenses/by-nc-nd/4.0/>).

nanoelectronics and sensing technologies [17–20]. Their electronic band structures and transport properties enable efficient interaction with low-energy electromagnetic radiation, while their reduced dimensionality allows strong field confinement and tunable optical conductivity [21,22]. Furthermore, heterostructures and multilayer configurations based on these materials can offer additional degrees of freedom for engineering the optical response in the THz regime [20,23].

In particular, Tungsten diselenide (WSe_2) has been extensively investigated due to its direct bandgap in the ML form and strong excitonic effects; these properties make it efficient for optical absorption and emission processes across the visible and near-infrared spectral regions [24,25]. Platinum diselenide (PtSe_2), on the other hand, has recently become a promising member of the noble metal dichalcogenide family; PtSe_2 exhibits a thickness-dependent electronic structure that transitions from a semimetallic behavior in bulk form to a semiconducting state in ML form. This tunable electronic structure, along with high environmental stability, makes PtSe_2 especially interesting for electronic and optoelectronic applications [26,27]. Additionally, PtSe_2 has shown excellent performance in photodetection and sensing applications due to its broadband optical response and high carrier mobility [28].

Thanks to near-atomic thickness and strong in-plane covalent bonds in PtSe_2 and WSe_2 , these materials offer a new approach to building van der Waals (vdW) heterostructures [29–32]. Hence, different single or multi-layered TMDs, as well as heterostructures based on diverse TMDs, have been studied for their optoelectronic properties. The interface-induced Seebeck effect for the $\text{PtSe}_2/\text{PtSe}_2$ vdW structure was reported by Lee et al. [33], who also offered an efficient method for utilizing this material to create the large-area thermoelectric energy harvesting devices that are perfect thermoelectric platforms with high figures of merit. Qiao et al. [34] have investigated the electronic properties of $\text{PtSe}_2/\text{WS}_2$ vdW heterostructures and the optical absorption analysis showed that this heterostructure can efficiently capture solar energy and has good photocatalytic activity in the ultraviolet and visible light regions. In another study, Han et al. [35] have evaluated the PtSe_2/SiH heterojunction, investigated its structural, electronic and optical properties, and discussed its application in photocatalysis. According to projected density of state (PDOS) results, they have found that PtSe_2/SiH is a type-II band alignment. Moreover, the excellent absorption coefficient of the PtSe_2/SiH heterostructure spans the whole region of visible light and has a peak value of $3.34 \times 10^5 \text{ cm}^{-1}$. The band edge position of the heterojunction crossed the redox potential of water, indicating ability for photocatalytic water splitting. Another study presented a phototransistor based on a PtSe_2/Si heterostructure fabricated on a silicon-on-insulator substrate. The built-in electric field at the PtSe_2/Si junction enables efficient separation of photo-generated carriers. The device shows gate-tunable photoresponse across a broad spectral range and very fast response times (about 36 μs). These results highlight the potential of PtSe_2 heterostructures for high-performance optoelectronic and transistor devices [36]. Iqbal et al. [37] has evaluated the fabrication of single-layer WS_2 field-effect transistors (FETs) with improved electrical performance. The h-BN/ WS_2 /h-BN sandwich structure significantly enhanced the carrier mobility and device stability. The devices achieve electron mobility up to about $214 \text{ cm}^2/\text{Vs}$ at room temperature and about $486 \text{ cm}^2/\text{Vs}$ at 5 K, with an on/off current ratio of about 10^7 . The results demonstrate a promising approach for high-performance, air-stable 2D semiconductor devices for nanoelectronics and optoelectronics. In a similar study, the high-performance *p*-type FETs based on ML WSe_2 (about 0.7 nm thick) using chemically doped source/drain contacts and high- κ gate dielectrics have been reported. The devices show high hole mobility (about $250 \text{ cm}^2/\text{Vs}$), and an on/off ratio above 10^6 at room temperature. These outcomes demonstrated promising device architecture for high-performance *p*-type transistors [38]. Si et al. [39] have assessed the band alignment of $\text{MoS}_2/\text{WSe}_2$ heterojunction samples with the support of X-ray photoelectron spectroscopy and first-principles theory calculations. Accordingly, the improved photoelectrochemistry (PEC) performance of the

heterojunction photoanode was ascribed to the built-in electric field between MoS_2 and WSe_2 nanosheets, which promoted the photo-generated *e-h* pair separation and suppressed their recombination. This study has verified the PEC mechanism of $\text{MoS}_2/\text{WSe}_2$ heterojunction photoelectrodes, which is significant for the design of PEC devices based on TMD heterostructures. More, Zheng et al. [40] using experimental and theoretical results have illustrated the rich potential of the families of WSe_2 to control spin currents in 2D spintronic devices. They measured the spin-filtering effect in all-vdW heterostructures with WSe_2 barrier. Combining 2D-perpendicular magnetic anisotropy Fe_3GeTe_2 (FGT) with different thicknesses of WSe_2 , the FGT/ WSe_2 /FGT spin valve showed distinct charge and spin transport behavior. Moreover, the negative magnetoresistance of -4.3% could be inverted into positive magnetoresistance (up to $+25.8\%$) with decreasing the WSe_2 thickness.

Among such promising industrial applications for both materials, it is highly demanding to develop atomistic methodologies to explore such physical features, which will significantly broaden the application of 2D WSe_2 and PtSe_2 materials and their vdW interfaces. In this work, using hybrid density functional theory calculations, we proposed the interfaces made of $\text{WSe}_2/\text{PtSe}_2$ on mica substrate. The impact of stacking from 1 ML to 4 ML of PtSe_2 , in the heterostructure $1\text{MLWSe}_2/(\text{xMLs}) \text{PtSe}_2$, has been systematically investigated. More attention has been dedicated to evaluating the band gap properties, PDOS, HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital) as frontier molecular orbitals, and optical properties. The impact of the interfaced properties on the charge redistribution between the layers of $1\text{MLWSe}_2/(1-4 \text{ MLs}) \text{PtSe}_2$ vdW heterostructure has also been assessed by molecular projected self-consistent Hamiltonian (MPSH) calculations.

In this study, we will focus on prediction the electronic and optical properties of the WSe_2 and PtSe_2 structures for application in low-frequency THz amplification by constructing their vdWs heterostructure systems. The terahertz gap absence of effective, portable, and affordable sources and detectors is one of the major obstacles to THz technology's potential [41,42]. In this context, exploring emerging materials, such as 2D heterostructures, and integration methods, is attracting increasing attention. We are followed our previous studies regarding the exploring THz adsorption properties in 2D TMDs vdW material interfaces, such as SnSe_2 and SnSe [13,43], VSe_2 [16], $\text{PtSe}_2/\text{MoSe}_2$ [44], WSe_2 [45], and graphene [46,47]. An experimental and theoretical study work of Huang et al. [48], reveal that broad absorption features spanning 0.5–15 THz, associated with free-carrier dynamics and photon-to-phonon transitions for $\text{MoS}_2/\text{WSe}_2/\text{MoS}_2$ heterostructure. More, energy transfer of a vdW heterostructure formed by monolayers of WSe_2 and PtSe_2 has studied by steady-state photoluminescence (PL) and time-resolved transient absorption spectroscopy. The results showed that $\text{WSe}_2/\text{PtSe}_2$ interface facilitates efficient type-I energy/exciton transfer mechanisms that modify local dielectric properties and enhance nonlinear terahertz emissions [49]. Further, optical-pump terahertz-probe (OPTP) setups demonstrated sub-picosecond carrier relaxation and transient conductivity changes ideal for high-speed optoelectronics for bilayer of $2\text{MLPtSe}_2/\text{MoSe}_2$ and 3MLWSe_2 deposited on mica substrate [44]. While previous studies have investigated different properties of WSe_2 and PtSe_2 bulk materials and heterostructures, they often overlook the experimental characterizations and device level behaviours. However, a comprehensive simulation-based approach is fundamental to fully understanding the system's boundary conditions as well as evaluations the structural, electronic and optical properties of the interfaces in atomic scale, as we focus on this work.

2. Computational details

All DFT results presented have performed within the framework of the Quantum Atomistic ToolKit (QATK) code [50]. The Kohn–Sham (KS) expression [51,52] was addressed using the linear combinations of

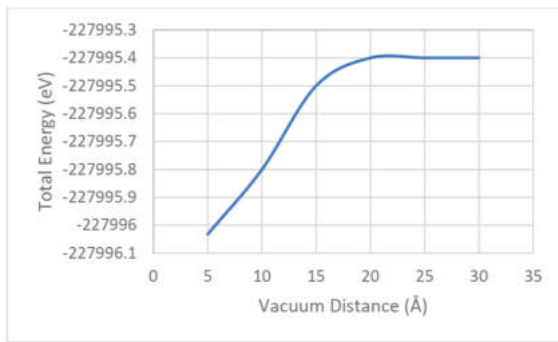


Fig. 1. Convergence tests for cutoff energy, k-point mesh, and vacuum thickness.

atomic orbitals (LCAO) basis set [53,54]. The HSE06 (Heyd-Scuseria-Ernzerhof) hybrid functional described the exchange-correlation functional, and the OMX pseudopotentials were used to approximate the wave functions in order to overcome the

drawbacks of conventional Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA) functionals [55]. In QuantumATK software, the use of scalar-relativistic HSE06 + spin-orbit coupling (SOC) it's not possible due to the software limitations and setup requirements. In this software, spin configurations are defined inside the calculator and script blocks via specific spin parameters of unpolarized, polarized (collinear), and noncollinear spin-orbit. Since we used LCAO basic set, by choosing HSE06 calculations, the LCAO calculator automatically reverts to unpolarized configurations. So, we cannot use the full noncollinear spin-orbit calculations with hybrid functionals natively. Furthermore, benchmark previous theoretical studies in the literature indicate that the fundamental band gap trends and the structural properties of TMDs materials and vdW interfaces can accurately be described by the HSE06 functional by introducing a portion of exact Fock (Hartree-Fock) exchange [56–61].

Since the vdW interactions, as the important forces, are not able to be correctly described by GGA calculations, we adopted the dispersion correction through parametrization developed by Grimme method (PBE-D3) [13,62]. The convergence tests for cutoff energy, k-point mesh, and vacuum thickness were performed for the mica/WSe₂/PtSe₂

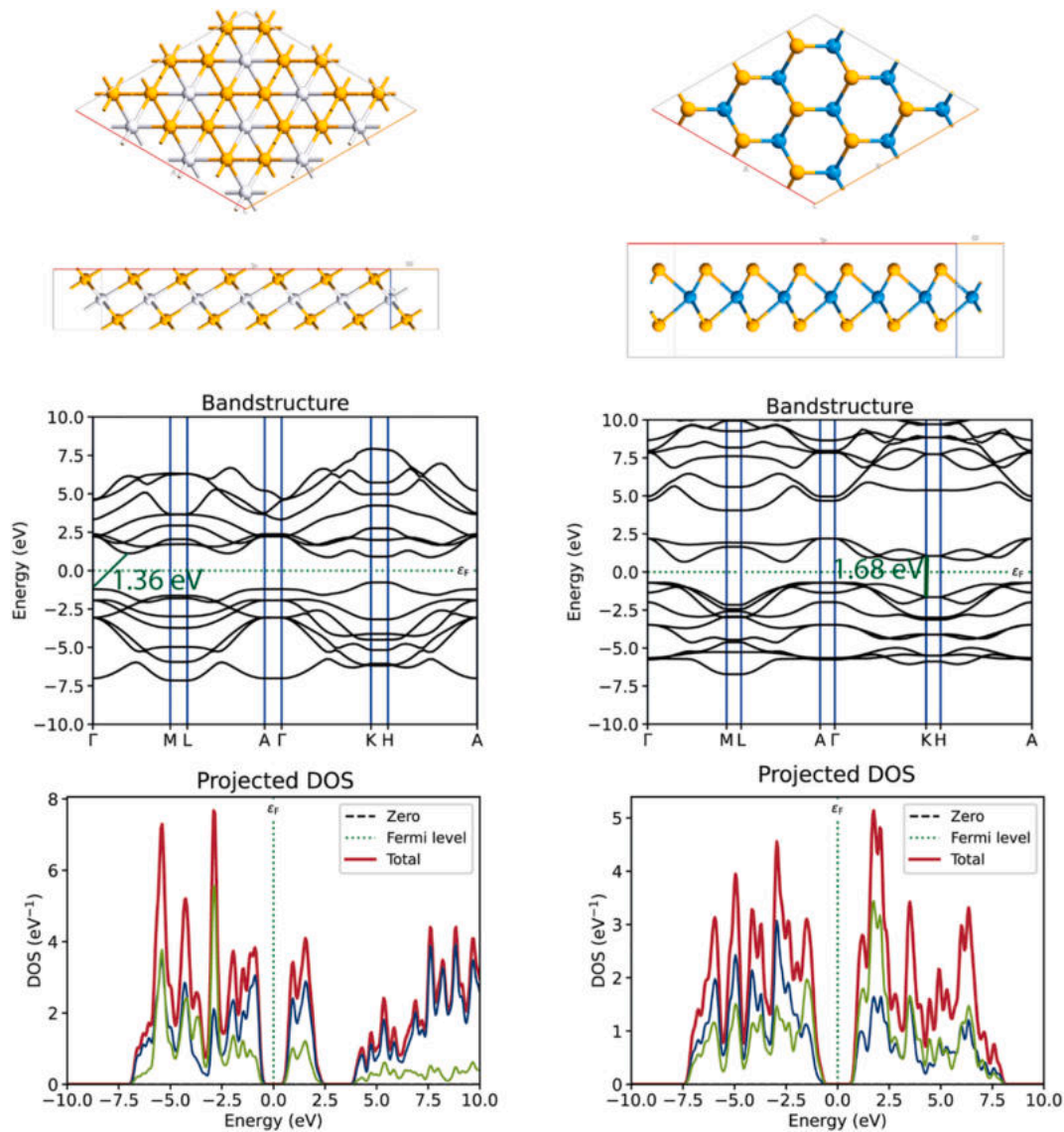


Fig. 2. Electronic properties of PtSe₂ and WSe₂ as a single layer. Schematic representation of both PtSe₂ and WSe₂, their respective band structure, and PDOS. The white, gold, and blue sticks are the Pt, Se, and W atoms, respectively. In the Projected Density of the State Pt and W are the represented as green curves, while Se is represented in the red curves, in both the systems respectively.

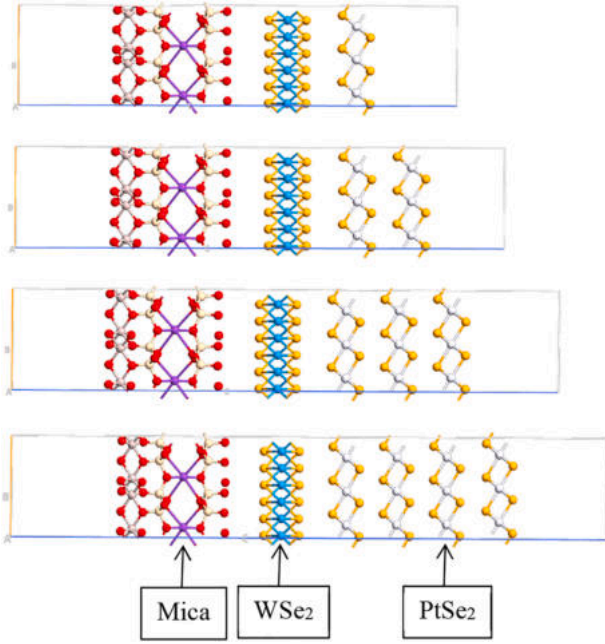


Fig. 3. The modelled geometries of 1MLWSe₂/(1-4 MLs) PtSe₂ on mica substrate; the white, gold and blue sticks are the Pt, Se and W atoms, respectively. The mica atoms coloured in O (red), Si (yellow), Al (brown), and P (violet), with H (white).

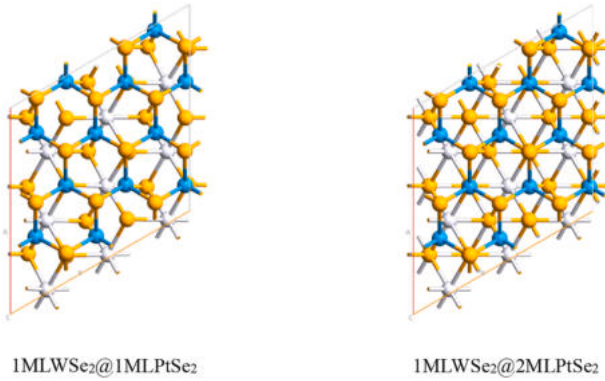


Fig. 4. Stacking configuration in a WSe₂/PtSe₂ vdW heterostructures; the white, gold and blue sticks are the Pt, Se and W atoms, respectively.

as the smallest heterostructure supercell, independently for each parameter, as seen in Fig. 1. Cutoff energy has tested from 10 Hartree to 130 Hartree. k-point mesh tests have calculated for total ground energy of the interface across mesh densities of $1 \times 1 \times 1$ up to $5 \times 5 \times 1$. Then, we considered the vacuum thickness variations, and we plotted the total energy as vacuum spacing increases from 5 Å to 30 Å to prove spurious electrostatic interactions between periodic images are eliminated.

A cutoff energy of 110 Ry was used, and geometries optimization were performed until the energy convergence satisfied the criterion of 1.0×10^{-6} eV/Å. The first Brillouin zone was sampled with the Monkhorst–Pack grid of $4 \times 4 \times 1$ k-points. The PDOS and band structure was calculated using a high k-point of $12 \times 12 \times 1$. To analyse the energy levels of HOMO-LUMO of different geometries, molecular projected self-consistent Hamiltonian (MPSH) calculations were executed.

The real part of the dielectric function ($Re(\omega)$), the imaginary part ($Im(\omega)$) and the absorption coefficient (α) are calculated by the following Formula [16,63,64],

$$\alpha_a = 2 \frac{\omega}{C} \kappa \quad (1)$$

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

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

where n and κ refer to complex refractive index (n) and extinction coefficient (κ), respectively. The $Im(\omega)$ 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,

$$n + i\kappa = \sqrt{\epsilon_r} \quad (4)$$

Also, the electron energy loss spectrum, can be described using the dielectric constants by,

$$L(\omega) = \frac{Re(\omega)^2}{Re(\omega)^2 + Im(\omega)^2} \quad (5)$$

3. Results and discussions

3.1. PtSe₂ and WSe₂ monolayer properties

The atomistic characterization of PtSe₂ and WSe₂ as individual systems represents the first step toward understanding the properties of layered hybrid structures based on these materials. PtSe₂, and WSe₂ are TMDs with a layered structure, in which the layers are stacked through vdW interactions, while strong covalent bonds hold the atoms together within each plane. The properties of the corresponding 2D MLs are of particular interest, as they exhibit electronic structures and optical behaviors distinct from those of their bulk counterparts. Here, PDOS and band structure were calculated to assess and validate the reliability of the proposed DFT methodology.

A PtSe₂ ML is characterized by a hexagonal crystal structure, where a central plane of Pt atoms is covalently bonded to two Se atomic layers located above and below it (Fig. 2). Its band structure reveals an indirect band gap of 1.36 eV, in good agreement with data reported in the literature [65,66]. The existence of the gap between valence and conduction bands, arising from contributions of both Pt and Se atoms, is also confirmed by the PDOS. Specifically, the PDOS shows that the high electronic states related to Se orbitals in the valence and conduction bands. A WSe₂ monolayer exhibits a direct band gap of 1.68 eV, with both the valence band maximum and the conduction band minimum located at the K point, while the bulk material has an indirect band gap of 0.94 eV [20,67]. The corresponding PDOS of WSe₂ originates from the W orbitals contributed in both the valence and conduction bands.

3.2. WSe₂/PtSe₂ vdW heterostructures on mica

After evaluating the monolayer systems properties, we simulated various interfaces of 1MLWSe₂/PtSe₂ on mica substrate by varying the PtSe₂ thicknesses, i.e. from one to four layers (Fig. 3). We included the mica substrate in our DFT models for some important reasons aimed at bridging the gap between theoretical modeling and experimental reality. Following our previous study for considering the carrier dynamics and electronic properties of PtSe₂/MoSe₂ and WSe₂ 2D layered structures on mica [44], this substrate is one of the most widely used materials for the experimental growth and exfoliation of 2D materials like WSe₂ and PtSe₂ due to its atomically flat surface [68]. We included the mica in our simulations ensures our calculations closely mimic realistic

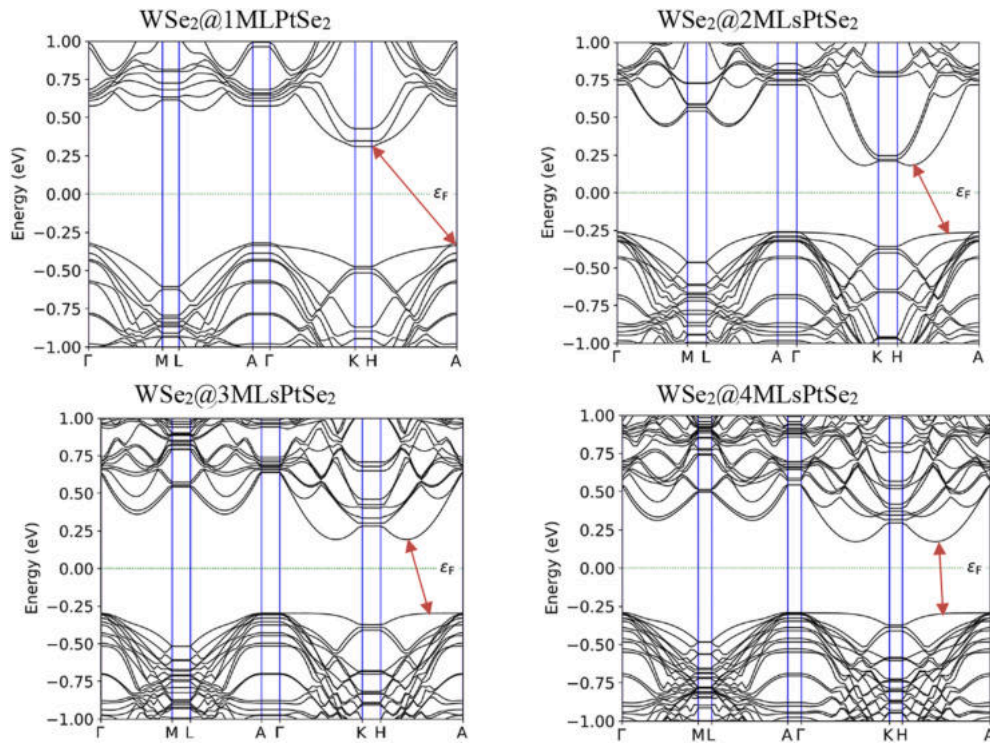


Fig. 5. DFT calculations on band structure variations of WSe₂ on multilayered PtSe₂. The relative positions of VBM and CBM with respect to Fermi level are inserted.

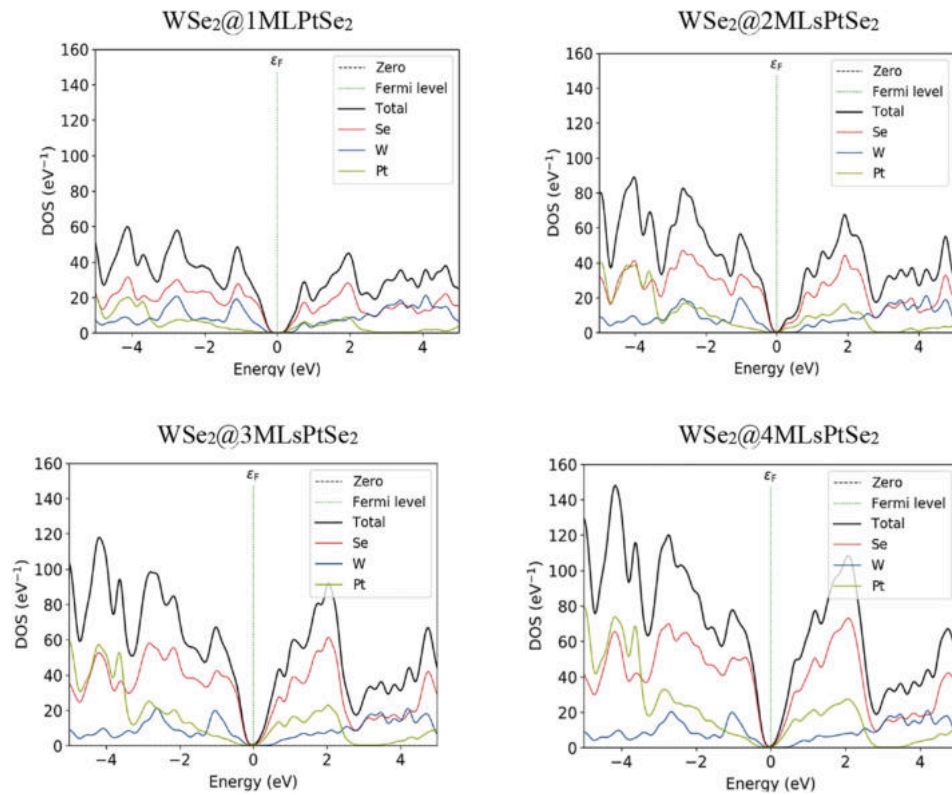


Fig. 6. PDOS calculations of WSe₂ on PtSe₂ different thicknesses.

experimental conditions to accurately account for substrate-induced lattice deformation and full geometry optimizations of WSe₂/PtSe₂ vdW heterostructures supported on the mica slab. However, after the optimization of the interfaces, we cut away the mica substrate from the

vdW heterostructures and the subsequent electronic structure and property calculations were carried out on the optimized freestanding TMDs layers to eliminate unphysical confinement or band-edge shifts from the wide-bandgap substrate and to focus exclusively on the

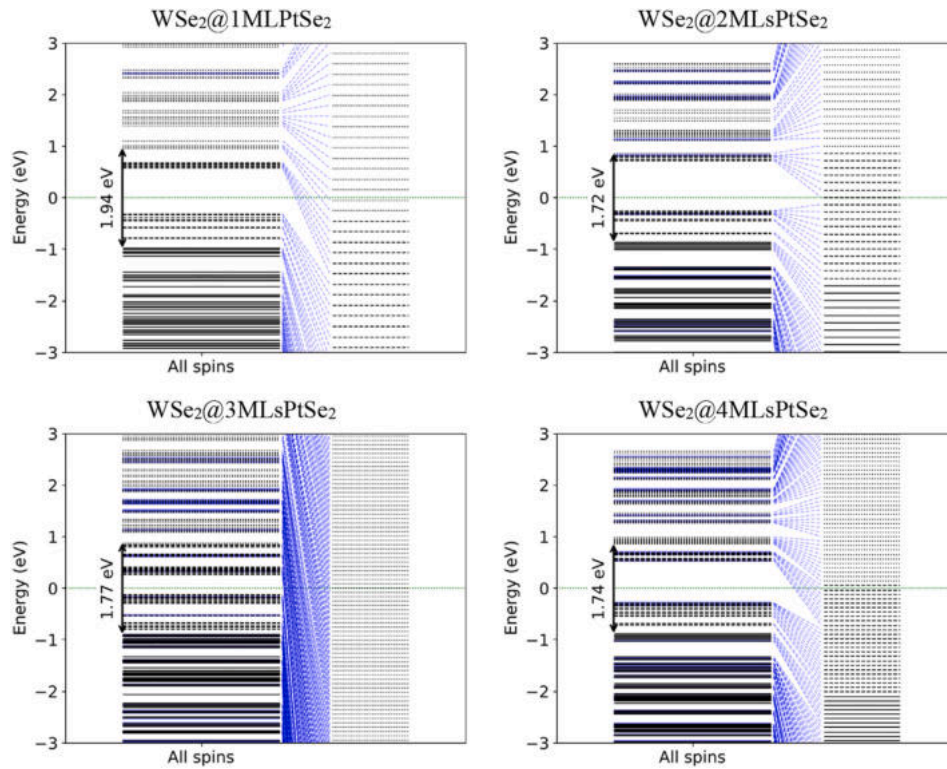


Fig. 7. MES calculations including the HOMO-LUMO band gaps and split energies of WSe₂ on PtSe₂ multilayers.

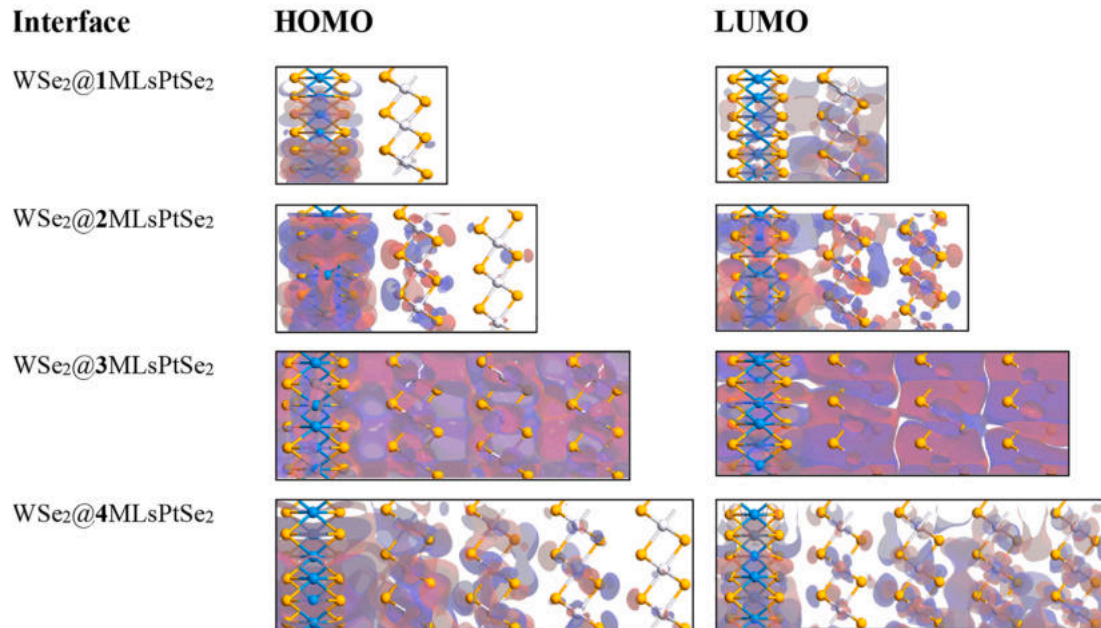


Fig. 8. Isosurfaces of HOMO and LUMO states of the WSe₂/(1-4 MLs)PtSe₂ interfaces.

intrinsic properties of the 2D TMDs layers. Then, 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 [69].

All lattices have been optimized with a minimum of 25 Å vacuum between the layer's periodic replica. The dimension of the supercells is $a = 10.41$ Å and $b = 10.44$ Å with the vary values of c axis by 38.84 Å,

42.99 Å, 46.23 Å, and 52.28 Å for mica/1MLWSe₂ on 1MLPtSe₂, 2MLPtSe₂, 3MLPtSe₂ and 4MLPtSe₂, respectively. The distance between the mica and the first layer of PtSe₂ (oxygen in the mica and Se in the PtSe₂) is 13 Å. All the supercells have hexagonal unit cells, as see in Fig. 4. While in the 2D hexagonal primitive unit cell, as a triangular grid configuration forming a 60° angle between the axes, in a 3D lattice form, the angles between the lattice axes are $\alpha = 90$, $\beta = 90^\circ$ and $\gamma = 120^\circ$.

Regarding to the stacking configuration of the WSe₂/1MLPtSe₂ heterostructure, as show in Figs. 3 and 4, exhibit the stacking AB

Table 1

HOMO and LUMO energy levels as well as the HOMO-LUMO band gaps of different interfaces of WSe₂/(1-4 MLs) PtSe₂.

Interface	HOMO-LUMO band gap (eV)	HOMO Energy (eV)	LUMO Energy (eV)
WSe ₂ @1MLPtSe ₂	1.94	-1.0687	0.8713
WSe ₂ @2MLsPtSe ₂	1.72	-0.9490	0.7710
WSe ₂ @3MLsPtSe ₂	1.77	-0.9803	0.7897
WSe ₂ @4MLsPtSe ₂	1.74	-0.9791	0.7609

configuration. The top WSe₂ monolayer shifts laterally relative to the bottom PtSe₂ monolayer. The W atoms sit in a trigonal prismatic coordination between the Se-Pt atoms. The WSe₂/2MLPtSe₂ stacked trilayer heterostructure can explicitly manifest as ABB stacking configuration (see Figs. 3 and 4). While the first layer (A) establishes the WSe₂ layer and the second layer (B) denotes as the middle layer PtSe₂, the third layer (B) implies that the top layer (PtSe₂) perfectly aligns with the middle layer (PtSe₂) without further lateral translation maintaining as homo-bilayer AA-like orientation between the two PtSe₂ sheets. Regarding to WSe₂/3MLPtSe₂ and WSe₂/4MLPtSe₂, simply have the stacking configurations of ABBB and ABBBB, respectively.

Then, we investigated the structural parameters once every superlattice had been fully optimized. About the mica/WSe₂/1MLPtSe₂, while the interlayer distance of mica-WSe₂ is around 3.68 Å, the alignment of 2D PtSe₂ with WSe₂ layers is accompanied by an initial vdW interlayer distance of around 3.13 Å between the individual layers. The vdW interlayer spacing has altered in mica-WSe₂ (3.57 Å), WSe₂-PtSe₂ (3.38 Å) and PtSe₂-PtSe₂ (3.62 Å) for WSe₂/2MLsPtSe₂, mica-WSe₂ (3.46 Å), WSe₂-PtSe₂ (3.60 Å) and PtSe₂-PtSe₂ (3.62 Å) for WSe₂/3MLsPtSe₂, and mica-WSe₂ (3.42 Å), WSe₂-PtSe₂ (3.55 Å) and PtSe₂-PtSe₂ (3.52 Å) for WSe₂/4MLsPtSe₂ due to an increase in PtSe₂ layer thickness.

We also considered the mica imposed biaxial strain on the WSe₂ and PtSe₂ monolayers. Since the mica surface cell dimension is

10.41 Å × 10.44 Å is match with 3×3 supercell of hexagonal monolayers, and the lattice constant (a) of WSe₂ and PtSe₂ calculated in this study are 3.28 Å and 3.74 Å, respectively, the imposed biaxial strain is calculated as:

$$\varepsilon_i = \frac{\varepsilon_{mica,i} - L_{layer}}{L_{layer}} \quad (6)$$

And $L_{layer} = 3a$,

Thus, for $a_{WSe_2} = 3.28$ Å, along the two mica directions: $\varepsilon_x = 5.79$ % and $\varepsilon_y = 6.10$ %, and the mica imposed approximately $\varepsilon_{WSe_2} \approx 5.95$ % average tensile strain in 3×3 WSe₂ cell.

For $a_{PtSe_2} = 3.74$ Å, along the two mica directions: $\varepsilon_x = -7.22$ % and $\varepsilon_y = -6.95$ %. The average imposed strain is therefore $\varepsilon_{PtSe_2} \approx -5.95$ % in 3×3 PtSe₂ cell, means that PtSe₂ is under compressive strain.

We also evaluated the direct lattice mismatch of the WSe₂/PtSe₂ interface. Using the primitive lattice constants and taking the WSe₂ as the reference;

Table 2

Optical adsorption properties along the in-plane and out-of-plane directions for all the interfaces of WSe₂/(1-4 MLs)PtSe₂.

Interface	In-plane direction			Out-of-plane direction
Frequency	12 THz	24 THz	36 THz	48 THz
WSe ₂ @1MLsPtSe ₂	660 cm ⁻¹	1798 cm ⁻¹	2329 cm ⁻¹	327 cm ⁻¹
WSe ₂ @2MLsPtSe ₂	3740 cm ⁻¹	7630 cm ⁻¹	9342 cm ⁻¹	982 cm ⁻¹
WSe ₂ @3MLsPtSe ₂	3776 cm ⁻¹	9194 cm ⁻¹	11,662 cm ⁻¹	3683 cm ⁻¹
WSe ₂ @4MLsPtSe ₂	2996 cm ⁻¹	7286 cm ⁻¹	9678 cm ⁻¹	7811 cm ⁻¹

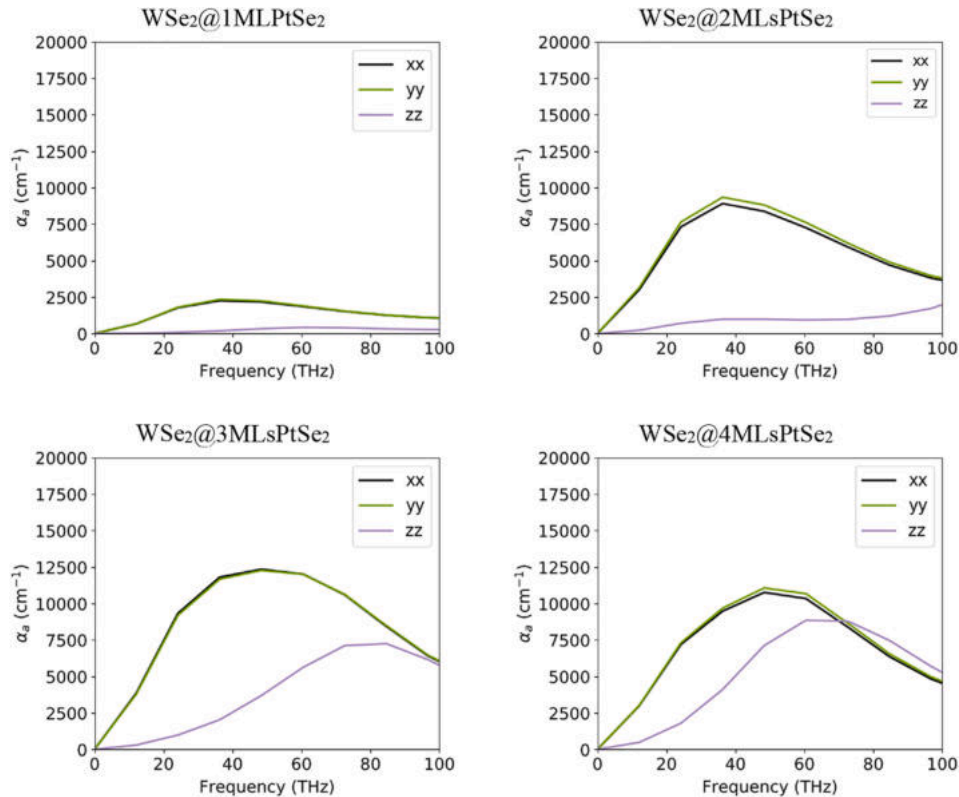


Fig. 9. Optical adsorption properties of the WSe₂/(1-4 MLs)PtSe₂ interfaces.

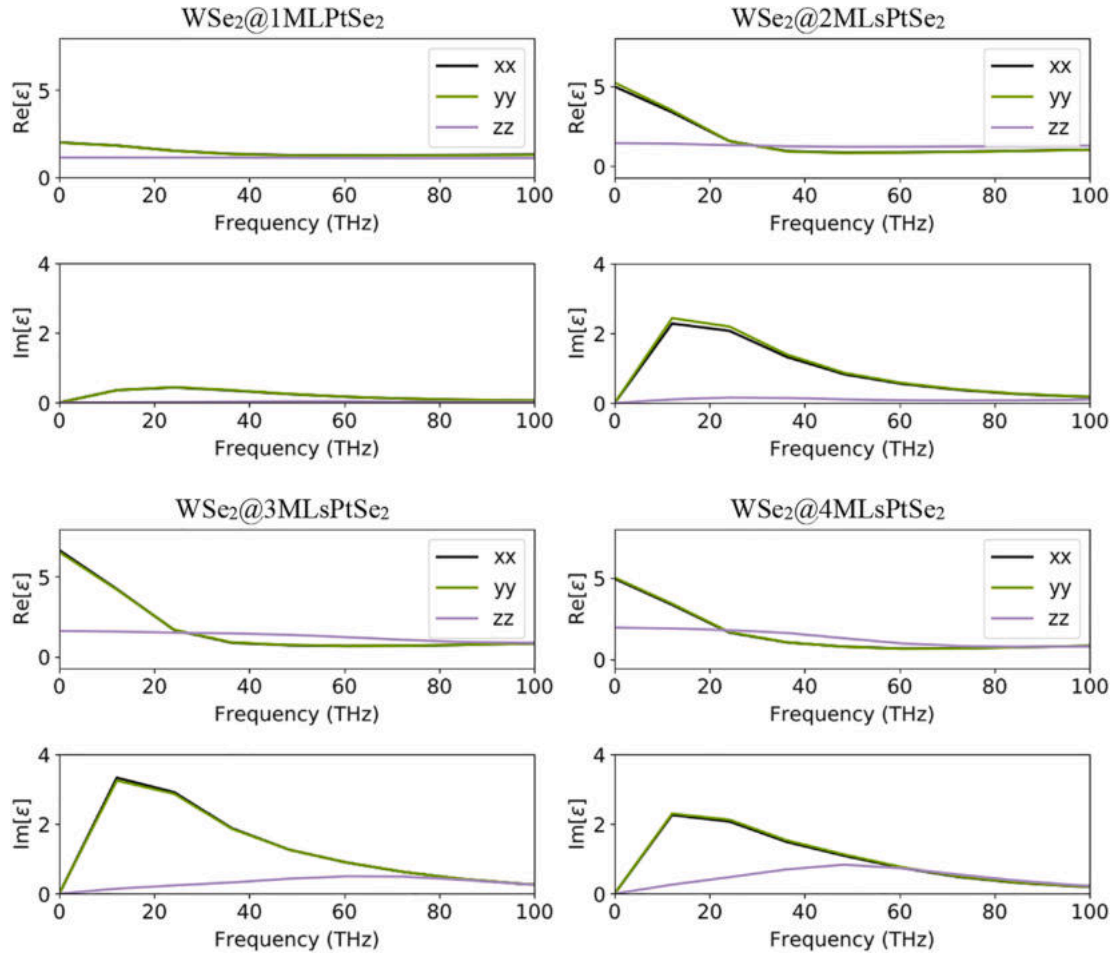


Fig. 10. Real (Re $[\epsilon]$) and imaginary (Im $[\epsilon]$) part of dielectric constant of the $\text{WSe}_2/(1-4 \text{ MLs})\text{PtSe}_2$ interfaces.

$$\delta = \frac{a_{\text{PtSe}_2} - a_{\text{WSe}_2}}{a_{\text{WSe}_2}} \quad (7)$$

The $\text{WSe}_2/\text{PtSe}_2$ calculated lattice mismatch is 14.02 %.

To evaluate the systems stability, the interlayer binding energy (E_B) of the mica/ $\text{WSe}_2/\text{PtSe}_2$ superlattices has been calculated as Eq. (8) [13],

$$E_B = \frac{E(\text{superlattice}) - E(\text{Mica}) - E(\text{WSe}_2) - nE(\text{PtSe}_2)}{N} \quad (8)$$

where $E(\text{superlattice})$ refers to total energy of superlattices of different thicknesses, $E(\text{Mica})$, $E(\text{WSe}_2)$ and $E(\text{PtSe}_2)$ are the total energy of the mica and material monolayers, n is the number of the PtSe_2 layers and N is the numbers of atoms in the supercells. The calculated E_B has obtained to be -0.162 eV/atom, -0.152 eV/atom, -0.143 eV/atom and -0.122 eV/atom for $\text{WSe}_2/1\text{MLPtSe}_2$, $\text{WSe}_2/2\text{MLPtSe}_2$, $\text{WSe}_2/3\text{MLPtSe}_2$, and $\text{WSe}_2/4\text{MLPtSe}_2$, respectively.

We theoretically explored the band structures of the WSe_2 @layered PtSe_2 (1-4 MLs) after optimizing the full structures based on DFT calculations (Fig. 5). The atomistic outcomes revealed that the semiconductor properties of all the interfaces with transition from an indirect to direct band gap by increasing the number of PtSe_2 layers. The simplest model of $\text{WSe}_2/1\text{MLPtSe}_2$ exhibited an indirect band gap of 627 meV with valence band maximum (VBM) ($E_{\text{VBM}} = -323$ meV) and conduction band minimum (CBM) ($E_{\text{CBM}} = 307$ meV). By increasing the thickness of the PtSe_2 from 1 ML to 4 MLs, the E_{VBM} of $\text{WSe}_2/2$ MLs PtSe_2 , $\text{WSe}_2/3$ MLs PtSe_2 and $\text{WSe}_2/4$ MLs PtSe_2 have slightly changed to -260 meV, -298 meV and -293 meV, respectively. The corresponding E_{CBM} are estimated to be 178 meV, 190 meV and 170 meV,

respectively, which minimise the band gaps in the interfaces with even layers of PtSe_2 from 438 eV in $\text{WSe}_2/2\text{MLsPtSe}_2$ to 488 eV in $\text{WSe}_2/3\text{MLsPtSe}_2$ and 463 eV for $\text{WSe}_2/4\text{MLsPtSe}_2$.

To further elucidate the interfacial charge interactions, we analysed the PDOS calculations of the $\text{WSe}_2/\text{PtSe}_2$ heterostructures as a function of the PtSe_2 layer thickness (Fig. 6). Analysis of the PDOS reveals that Se atoms dominate the DOS across all interfaces, exhibiting prominent peaks both just below and above the Fermi level. In the E_{VBM} region, W displays the next highest DOS contribution. As the number of PtSe_2 layers increases, our theoretical results reveal a distinct atomic competition in the valence band: the W (5d) and Pt (5d) orbitals begin to overlap and compete for dominance. Conversely, in the E_{CBM} region, Pt atoms consistently provide the second-highest DOS (after Se). As the PtSe_2 thickness increases, the Se, Pt and W atomic-derived DOS increases across all evaluated interfaces, indicating enhanced interlayer electron delocalization. In agreement to the band structure calculations of different interfaces, the total PDOS increasing at the E_{VBM} and E_{CBM} regions cause the strong interfacial coupling and charge redistribution as well as the tuning of the band alignment from indirect to direct band gap. We mention that PtSe_2 exhibits a distinct layer-dependent evolution where its band gap changes significantly with thickness (Fig. 5).

It is worthy to notice that the vdWs interaction between layers in TMDs materials like MoSe_2 and WSe_2 alters the overlap of the out-of-plane P_z and in-plane $P_x + y$ orbitals of the Se atoms, because interfaces break translational symmetry in the out-of-plane direction, and the out-of-plane orbital hybridization undergoes a strong odd-even alternating effect [70–72]. In $\text{WSe}_2/\text{PtSe}_2$ heterostructures with odd-numbered layers, the lack of spatial inversion symmetry can lead to an uncompensated interface dipole. This built-in electric field breaks the

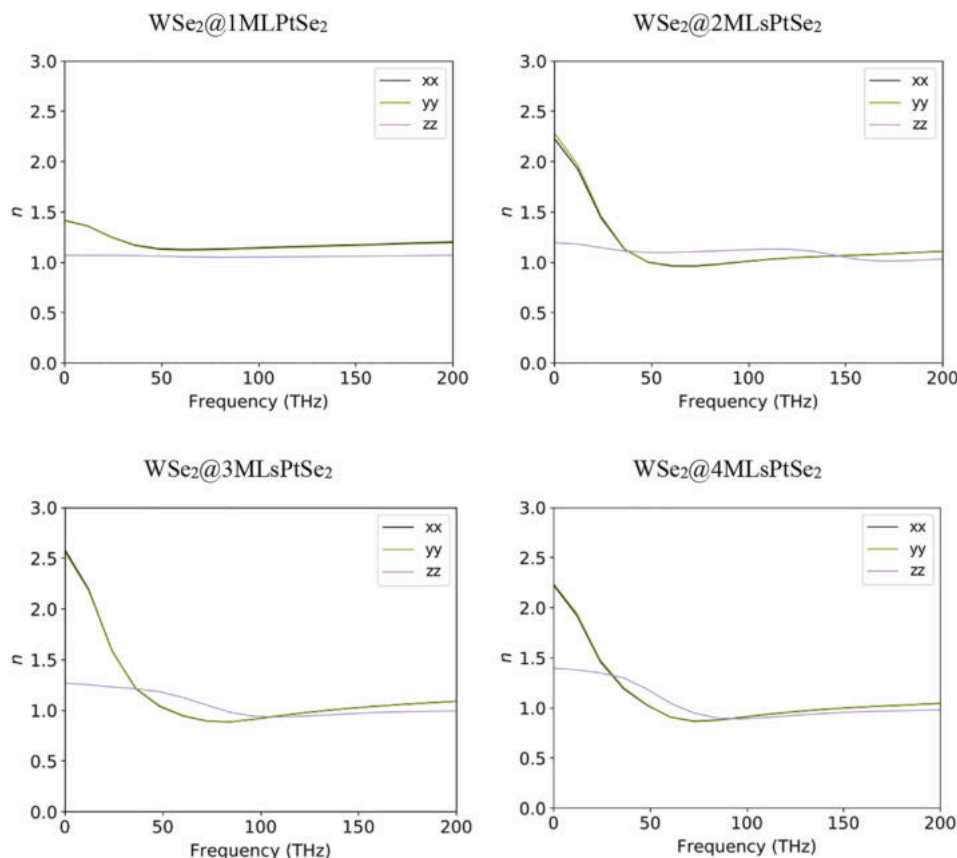


Fig. 11. Reflective index of the $\text{WSe}_2/(1-4 \text{ MLs})\text{PtSe}_2$ interfaces.

spatial symmetry of the confined electron states in the PtSe_2 layer, shifting the energy eigenvalues of the conduction and valence bands. Even-layer interfaces maintain better structural inversion symmetry, cancelling out these dipoles and creating a more homogeneous, delocalized charge distribution that narrows the band gap. As we discuss later in the HOMO-LUMO states, $\text{WSe}_2/\text{PtSe}_2$ and $\text{WSe}_2/3\text{PtSe}_2$ heterostructures will be shown this fact with more orbital delocalization between the layers.

The molecular energy spectrum and HOMO-LUMO energy splitting from MPSH calculations can be seen in Fig. 7 and Table 1, which demonstrates molecular spectrum energy and eigenstate energy levels of $\text{WSe}_2/(1-4 \text{ MLs})\text{PtSe}_2$ different interfaces. It has been predicted to have lower HOMO-LUMO band gap when there are the even layers of PtSe_2 in the interfaces of 1.72 eV and 1.74 eV for $\text{WSe}_2/2 \text{ MLsPtSe}_2$ and $\text{WSe}_2/4 \text{ MLsPtSe}_2$, respectively, while $\text{WSe}_2/1 \text{ MLsPtSe}_2$ and $\text{WSe}_2/3 \text{ MLsPtSe}_2$ with the odd layers of PtSe_2 showed higher band gap energy of 1.94 eV and 1.77 eV, respectively (see Fig. 8).

The HOMO-LUMO isosurfaces from MPSH can be seen in Fig. 6, demonstrating the charge density redistribution and eigenstate energy levels of $\text{WSe}_2/(1-4 \text{ MLs})\text{PtSe}_2$ systems. The HOMO energy value decreased from -0.1247 eV in $\text{WSe}_2/1 \text{ MLPtSe}_2$ to -0.2990 eV in $\text{WSe}_2/2 \text{ MLsPtSe}_2$, then increased to -0.1420 eV in $\text{WSe}_2/3 \text{ MLsPtSe}_2$ and ultimately reached -0.3061 eV in $\text{WSe}_2/4 \text{ MLsPtSe}_2$, according to the variation of the eigenstates in the region below the E_F . While the $\text{WSe}_2/1 \text{ MLPtSe}_2$ and $\text{WSe}_2/4 \text{ MLsPtSe}_2$ have the same LUMO energy level of 0.2734 eV, $\text{WSe}_2/2 \text{ MLsPtSe}_2$ and $\text{WSe}_2/3 \text{ MLsPtSe}_2$ showed an increase in the LUMO energy to 0.7156 eV and 0.5409 eV, respectively. In conclusion, the interfaces with the odd layers of PtSe_2 , particularly the $\text{WSe}_2/3 \text{ MLsPtSe}_2$, show a reduced HOMO-LUMO band gap because the charge density in the molecular orbitals of all the layers in contact is completely delocalized.

Optical absorption spectra for different interfaces of $\text{WSe}_2/$

1 MLPtSe_2 , $\text{WSe}_2/2 \text{ MLsPtSe}_2$, $\text{WSe}_2/3 \text{ MLsPtSe}_2$, and $\text{WSe}_2/4 \text{ MLsPtSe}_2$ have been then compared, as a function of Frequency (THz), as reported in Fig. 9. The main first peak was positioned at 12 THz, 24 THz, and 36 THz along the in-plane direction for all the interfaces with different intensities of the adsorption coefficient (see Table 2). The adsorption intensity did not exhibit a regular pattern, according to the DFT-data; however, $\text{WSe}_2/3 \text{ MLsPtSe}_2$ showed the structure with the highest adsorption intensity. Indeed, the corresponding adsorption peaks of four interfaces along the out-of-plane shown a consistent trend, i.e. by increasing the PtSe_2 thickness, the peaks shifted to the lower THz frequencies, and the intensity of the optical adsorption has enhanced (see the frequencies in 48 THz, including Table 2).

The data presented in Fig. 10 deal with the dielectric functions directly calculated by the DFT packages. The real part ($\text{Re}(\omega)$) of dielectric function, which is related to the static dielectric constant, shown positive values for all the interfaces with $\text{WSe}_2/1 \text{ MLPtSe}_2$ (in-plane = 1.98 and out-of-plane = 1.13), $\text{WSe}_2/2 \text{ MLsPtSe}_2$ (in-plane = 5.20 and out-of-plane = 1.41), $\text{WSe}_2/3 \text{ MLsPtSe}_2$ (in-plane = 6.54 and out-of-plane = 1.59), and $\text{WSe}_2/4 \text{ MLsPtSe}_2$ (in-plane = 5.00 and out-of-plane = 1.93). These results indicate that the total reflectance of photon-electron interaction in the light polarization along the in-plane is larger than the out-of-plane direction.

Based on Fig. 10 for $\text{WSe}_2/(1-4 \text{ MLs})\text{PtSe}_2$ interfaces, the absorption edge of $\text{Im}(\omega)$, which was equal to the optical gap, located at zero along the in-plane and out-of-plane directions in all the structures. Our atomistic results revealed that $\text{WSe}_2/3 \text{ MLsPtSe}_2$ has higher peak intensity along the in-plane direction in the frequency of 24 THz, while $\text{WSe}_2/1 \text{ MLPtSe}_2$ possess the lowest one. The first main peak of $\text{Im}(\omega)$ along the out-of-plane polarization shown more intensity by increasing the PtSe_2 thickness.

Figs. 11 and 12 show the refractive index and extinction coefficient of different interfaces of $1 \text{ MLWSe}_2/(1-4 \text{ MLs})\text{PtSe}_2$. From Fig. 11, the

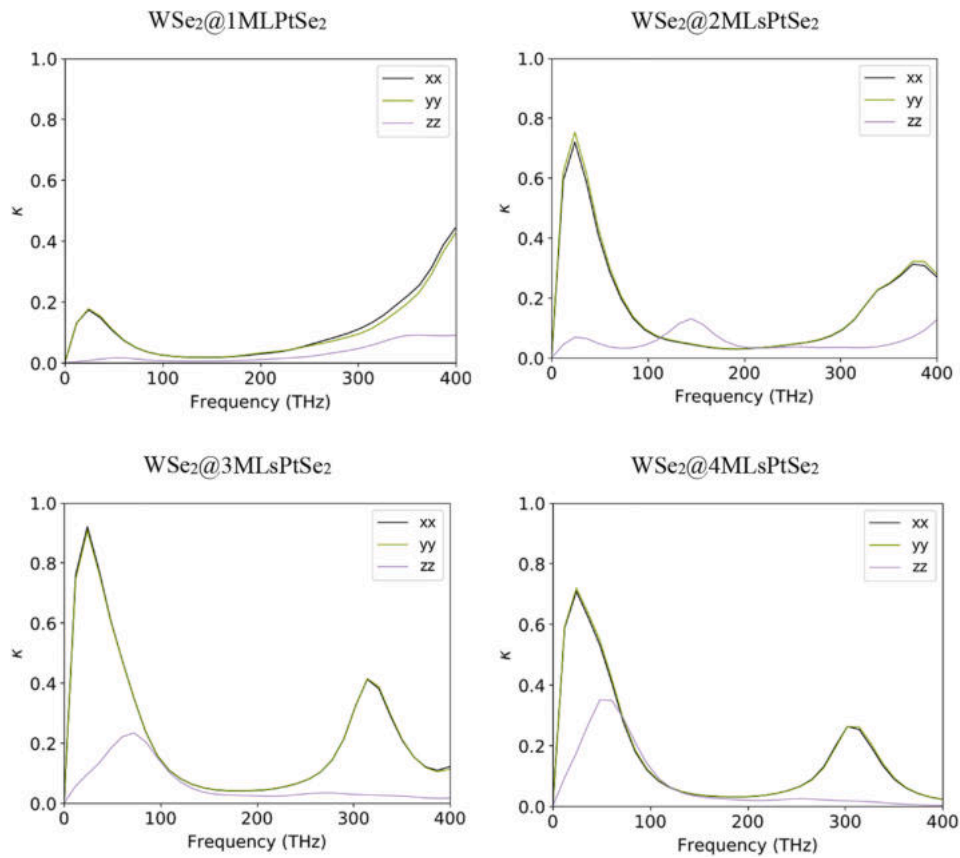


Fig. 12. Extinction coefficient of the $\text{WSe}_2/(1-4 \text{ MLs})\text{PtSe}_2$ interfaces.

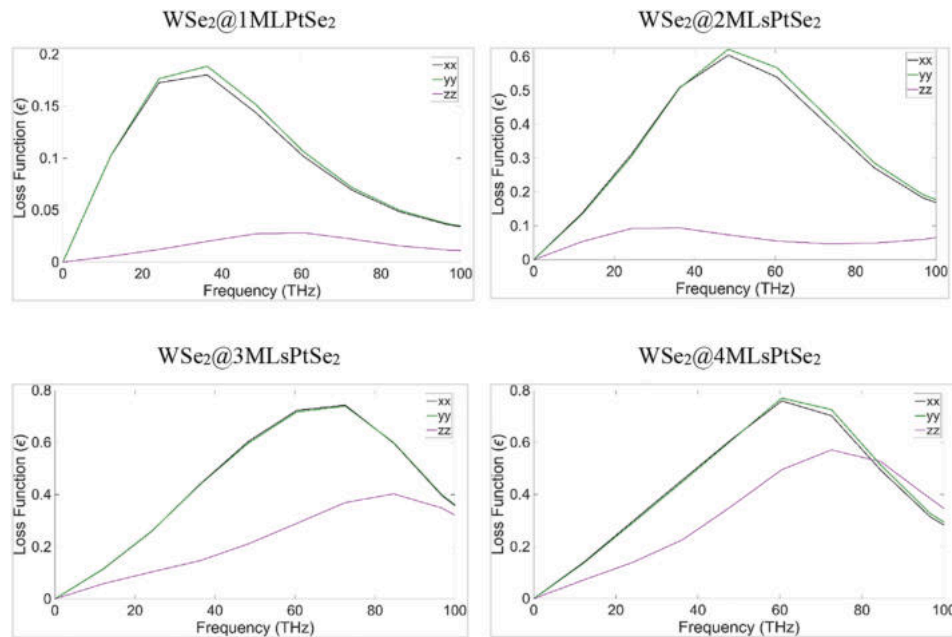


Fig. 13. Energy loss function spectra for the $\text{WSe}_2/(1-4 \text{ MLs})\text{PtSe}_2$ interfaces.

static refractive indices were 1.41, 2.28, 2.55, and 2.23 in the in-plane direction for $\text{WSe}_2/1\text{MLPtSe}_2$, $\text{WSe}_2/2\text{MLsPtSe}_2$, $\text{WSe}_2/3\text{MLsPtSe}_2$, and $\text{WSe}_2/4\text{MLsPtSe}_2$, respectively. Along the out-of-plane, the static refractive indices have increased from 1.06 in $\text{WSe}_2/1\text{MLPtSe}_2$ to 1.19, 1.26 and 1.39 for $\text{WSe}_2/2\text{MLsPtSe}_2$, $\text{WSe}_2/3\text{MLsPtSe}_2$, and $\text{WSe}_2/4\text{MLsPtSe}_2$, respectively. The first peak values of the extinction

coefficients in Fig. 12 for $\text{WSe}_2/1\text{MLPtSe}_2$ (in-plane = 0.17 in 24 THz and out-of-plane = 0.02 in 48 THz), $\text{WSe}_2/2\text{MLsPtSe}_2$ (in-plane = 0.75 in 24 THz and out-of-plane = 0.06 in 24 THz), $\text{WSe}_2/3\text{MLsPtSe}_2$ (in-plane = 0.90 in 24 THz and out-of-plane = 0.23 in 72 THz), and $\text{WSe}_2/4\text{MLsPtSe}_2$ (in-plane = 0.71 in 24 THz and out-of-plane = 0.35 in 48 THz).

The theoretical energy loss function presented in Fig. 13 shows the maximum energy loss peak at 38 THz, 49 THz, 71 THz, and 59 THz along the in-plane direction for $\text{WSe}_2/\text{1MLPtSe}_2$, $\text{WSe}_2/\text{2MLPtSe}_2$, $\text{WSe}_2/\text{3MLPtSe}_2$, and $\text{WSe}_2/\text{4MLPtSe}_2$, respectively. Since the imaginary part, $\text{Im}(\omega)$, of the dielectric function is related to the optical absorption properties of materials, it is predicted from the dielectric function spectra that $\text{WSe}_2/(1\text{--}4\text{ MLs})\text{PtSe}_2$ interfaces has strong light absorption in a wide range of photon energy in the range of 0–100 Frequency (THz). The results reveal that we can tune both the optical and electronic properties of $\text{WSe}_2/\text{PtSe}_2$ structure by varying the PtSe_2 thickness.

We compared the optical properties of $\text{WSe}_2/\text{PtSe}_2$ vdW interface systems in this study with the experimental refractive index (n) and extinction coefficient (k) of the $\text{1MLMoSe}_2/\text{2MLPtSe}_2$ from our previous work [44] fabricated on the mica substrate. The outcomes reveal that this interface does not introduce any observable optical absorption as simulated in the theoretical calculations. Thus, effective k is also almost zero similar to what we predicted for the $\text{WSe}_2/(1\text{--}4\text{ MLs})\text{PtSe}_2$ response. More, 1 ML $\text{MoSe}_2/2\text{ MLs PtSe}_2$ showed the maximum reflective index at 2.75 a bit higher than $\text{WSe}_2/\text{3MLPtSe}_2$ with the value of 2.55 along the in-plane direction. It worthy to notice that this study suggested a significant improvement in the optical properties of $\text{WSe}_2/\text{PtSe}_2$ vdW interfaces with respect to the $\text{WSe}_2/\text{HfSe}_2$ heterostructure in Ref. [73], by shifting the first adsorption peaks from visible light to infrared spectrum due to lower optical band gap. Regarding to adsorption coefficient of both interfaces, whereas the intensity of $\text{WSe}_2/\text{HfSe}_2$ can reach to $\approx 700,000\text{ cm}^{-1}$, $\text{WSe}_2/\text{3MLPtSe}_2$ has exhibited the lower adsorption intensity of $12,500\text{ cm}^{-1}$. The optical absorption coefficient in the orders of $10,000\text{ cm}^{-1}$ is very favorable for solar energy harvesting [74,75].

4. Conclusion

In this work, we used a DFT approach to investigate monolayers of PtSe_2 and WSe_2 as separate entities, and their multilayer heterostructures based on 1 ML WSe_2 combined with 1–4 MLs of PtSe_2 . The calculated band structures of the isolated monolayers confirm the reliability of the computational methodology, reproducing the expected indirect bandgap of PtSe_2 and the direct bandgap of WSe_2 . When the monolayer systems were assembled into vdW heterostructures, the electronic properties are significantly modified by the number of PtSe_2 layers. Interestingly, the heterostructure calculations showed a semi-conducting behavior with a reduction of the bandgap for the interfaces with odd layers of PtSe_2 , and a progressive transition toward a direct bandgap as the number of PtSe_2 layers has increased.

The PDOS analysis showed that Se orbital states contributed strongly to both valence and conduction portions, while a competition has occurred between Pt and W in the valence band by influence from the layer thickness. This indicates that the interfacial electronic structure can be tuned through layer engineering. In addition, the MPSH results revealed a redistribution and delocalization of the frontier orbitals, with the $\text{WSe}_2/\text{3MLPtSe}_2$ system showing that the charge density in the molecular orbitals is completely delocalized. In addition, the calculated optical absorption in the range of Frequency (THz) confirms the strong dependence of the optical response on PtSe_2 thickness, with an in-plane absorption that is maximized for $\text{WSe}_2/\text{3MLPtSe}_2$. Further, other optical characteristics revealed that higher peak intensity in the $\text{Im}(\omega)$ as well as static dielectric constant. These findings show that PtSe_2 thickness may efficiently adjust the band structure, electrical characteristics, THz optical response, and dielectric constant of $\text{1MLWSe}_2/(1\text{--}4\text{ MLs})\text{PtSe}_2$, paving the path for these layered systems in upcoming THz optoelectronic applications.

In summary, our study maps the primary finding related to the structure properties, electronic band structures and optical properties of the investigated $\text{1MLWSe}_2/(1\text{--}4\text{ MLs})\text{PtSe}_2$ vdW heterostructures. To build upon these insights, the immediate next step requires experimental

measurements to validate our theoretical predictions. Specifically, utilizing photoluminescence spectroscopy and Angle-Resolved Photoemission Spectroscopy (ARPES) measurements will be crucial to confirm the predicted properties. Furthermore, a comprehensive evaluation demands the consideration of other key properties such as thermal conductivity, mechanical stability, carrier mobility, lifetime, and contact effects, to ensure these materials can withstand the operational demands of next-generation optoelectronic devices.

CRediT authorship contribution statement

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

Declaration of competing interests

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.

Acknowledgments

This work is part of the research of HORIZON-EIC-2022-PATHFINDEROPEN-01 “Nano-scale Development of Plasmonic Amplifiers Based on 2D Materials” (PLASNANO) (grant agreement No. 101099552).

Data availability

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

References

- [1] Heffernan, B.M., Kawamoto, Y., Maekawa, K., Greenberg, J., Amin, R., Hori, T., Tanigawa, T., Nagatsuma, T., Rolland, A., 2023. 60 Gbps real-time wireless communications at 300 GHz carrier using a Kerr microcomb-based source. *APL Photonics* 8. <https://doi.org/10.1063/5.0146957/2897308>.
- [2] Sengupta, K., Nagatsuma, T., Mittleman, D.M., 2018. Terahertz integrated electronic and hybrid electronic–photonic systems. *Nat. Electron.* 1 (12), 622–635. <https://doi.org/10.1038/s41928-018-0173-2>, 1 (2018).
- [3] Agarwal, A., Pickwell-MacPherson, E., 2026. Past, present and future of in vivo THz skin sensing. *J. Phys.: Photonics* 8, 011001.
- [4] Chamola, V., Peelam, M.S., Guizani, M., Niyato, D., 2025. Future of connectivity: a comprehensive review of innovations and challenges in 7g smart networks. *IEEE Open Journal of the Communications Society* 6, 3555–3613.
- [5] Sundaravadivazhagan, B., Gnanasankaran, N., Raj, P., Raja, A.S., 2025. Virtual Reality and Augmented Reality with 6G Communication. John Wiley & Sons.
- [6] Julien, K.B., 2025. 6G wireless networks and terahertz communications: intelligent reflecting surfaces, MIMO, and energy-efficient IoT architectures. *World* 25, 1712–1736.
- [7] Baduge, G.A., Vaezi, M., Dassanayake, J.K., Hameed, M.Z., Ollila, E., Vorobyov, S. A., 2025. Frequency Range 3 for ISAC in 6G: Potentials and Challenges. *ArXiv Preprint ArXiv:2506.18243*.
- [8] Jia, S., Lo, M.C., Zhang, L., Ozolins, O., Udalcovs, A., Kong, D., Pang, X., Guzman, R., Yu, X., Xiao, S., Popov, S., Chen, J., Carpintero, G., Morioka, T., Hu, H., Oxenlowe, L.K., 2022. Integrated dual-laser photonic chip for high-purity carrier generation enabling ultrafast terahertz wireless communications. *Nat. Commun.* 13 (1), 1388. <https://doi.org/10.1038/s41467-022-29049-2>, 13 (2022).
- [9] Ukirade, N.A., 2025. A review on advancement of materials for terahertz applications. *Next Mater.* 6, 100479.
- [10] Samaha, A., Doumani, J., Kritzell, T.E., Xu, H., Baydin, A., Ajayan, P.M., El Tahchi, M., Kono, J., 2025. Graphene terahertz devices for sensing and communication. *Small* 21, 2401151.

- [11] Low, T., Avouris, P., 2014. Graphene plasmonics for terahertz to mid-infrared applications. *ACS Nano* 8, 1086–1101. https://doi.org/10.1021/NN406627U/ASSET/IMAGES/LARGE/NN-2013-06627U_0009.JPEG.
- [12] Tonouchi, M., 2007. Cutting-edge terahertz technology. *Nat. Photonics* 1 (2), 97–105. <https://doi.org/10.1038/nphoton.2007.3>, 1 (2007).
- [13] Mohebbi, E., Pavoni, E., Pierantoni, L., Stipa, P., Zampa, G.M., Laudadio, E., Mencarelli, D., 2024. Band gap and THz optical adsorption of SnSe and SnSe₂ nanosheets on graphene: negative dielectric constant of SnSe. *Results Phys.*, 107415.
- [14] Cheng, R., Li, D., Zhou, H., Wang, C., Yin, A., Jiang, S., Liu, Y., Chen, Y., Huang, Y., Duan, X., 2014. Electroluminescence and photocurrent generation from atomically sharp WSe₂/MoS₂ heterojunction p–n diodes. *Nano Lett.* 14, 5590–5597.
- [15] Wang, J., He, D., Bai, Z., Li, G., Bai, J., Liu, K., Ren, F., Liu, X., He, J., Zhou, W., 2023. Enhanced exciton diffusion from interlayer charge-transfer transitions in PtSe₂/MoSe₂ van der Waals heterojunction. *Nano Res.* 16, 12809–12816.
- [16] Mohebbi, E., Pavoni, E., Stipa, P., Pierantoni, L., Laudadio, E., Mencarelli, D., 2025. Tunable optical properties of Cu/VSe₂ from the visible to terahertz spectral range: a first-principles study. *Int. J. Mol. Sci.* 26, 2527.
- [17] Wang, Q.H., Kalantar-Zadeh, K., Kis, A., Coleman, J.N., Strano, M.S., 2012. Electronics and optoelectronics of two-dimensional transition metal dichalcogenides. *Nat. Nanotechnol.* 7 (11), 699–712. <https://doi.org/10.1038/nnano.2012.193>, 7 (2012).
- [18] Manzeli, S., Ovchinnikov, D., Pasquier, D., Yazyev, O.V., Kis, A., 2017. 2D transition metal dichalcogenides. *Nat. Rev. Mater.* 2 (8), 17033. <https://doi.org/10.1038/natrevmats.2017.33>, 2 (2017).
- [19] Chhowalla, M., Shin, H.S., Eda, G., Li, L.J., Loh, K.P., Zhang, H., 2013. The chemistry of two-dimensional layered transition metal dichalcogenide nanosheets. *Nat. Chem.* 5 (4), 263–275. <https://doi.org/10.1038/nchem.1589>, 5 (2013).
- [20] Aytekin, Y.S., Vergnaud, C., Sharma, R., Marty, A., Pavoni, E., Mohebbi, E., Laudadio, E., Jamet, M., Mencarelli, D., Altan, H., Esenturk, O., 2025. Ultrafast carrier dynamics and electronic properties of PtSe₂/MoSe₂ and WSe₂ 2D TMDC layered structures on mica: combined THz spectroscopy and DFT study. *RSC Adv.* 16, 425–438. <https://doi.org/10.1039/D5RA07084H>.
- [21] Widiyandari, H., Firdaus, I., Kadarisman, V.G.S., Purwanto, A., 2016. Optical properties and photocatalytic activities of tungsten oxide (WO₃) with platinum co-catalyst addition. In: *AIP Conf. Proc.* AIP Publishing LLC, 050027.
- [22] Unikandanunni, V., Rigoni, F., Hoffmann, M.C., Vavassori, P., Urazhdin, S., Bonetti, S., 2022. Ultrafast electron dynamics in platinum and gold thin films driven by optical and terahertz fields. *Appl. Phys. Lett.* 120.
- [23] Novoselov, K.S., Mishchenko, A., Carvalho, A., Castro Neto, A.H., 2016. 2D materials and van der Waals heterostructures. *Science* 353. https://doi.org/10.1126/SCIENCE.AAC9439/ASSET/4B54077E-FOA2-4BB2-BFA1-BC557DC78A9D/ASSETS/GRAPHIC/353.AAC9439_F6.JPEG, 1979.
- [24] Zhao, W., Ghorannevis, Z., Chu, L., Toh, M., Kloc, C., Tan, P.H., Eda, G., 2013. Evolution of electronic structure in atomically thin sheets of ws 2 and wse2. *ACS Nano* 7, 791–797. https://doi.org/10.1021/NN305275H/SUPPL_FILE/NN305275H_SI_001.PDF.
- [25] Fang, H., Chuang, S., Chang, T.C., Takei, K., Takahashi, T., Javey, A., 2012. High-performance single layered WSe 2 p-FETs with chemically doped contacts. *Nano Lett.* 12, 3788–3792. https://doi.org/10.1021/NL301702R/SUPPL_FILE/NL301702R_SI_001.PDF.
- [26] Kandemir, A., Akbal, B., Kahraman, Z., V Badalov, S., Ozcan, M., İyikanat, F., Sahin, H., 2018. Structural, electronic and phononic properties of PtSe₂: from monolayer to bulk, semicond. *Sci. Technol.* 33, 085002.
- [27] Wang, Y., Pang, J., Cheng, Q., Han, L., Li, Y., Meng, X., Ibarlucea, B., Zhao, H., Yang, F., Liu, H., 2021. Applications of 2D-layered palladium diselenide and its van der Waals heterostructures in electronics and optoelectronics. *Nano-Micro Lett.* 13, 143.
- [28] Wang, G., Wang, Z., McEvoy, N., Fan, P., Blau, W.J., 2021. Layered PtSe₂ for sensing, photonic, and (opto-) electronic applications. *Adv. Mater.* 33, 2004070.
- [29] Wu, R., Tao, Q., Dang, W., Liu, Y., Li, B., Li, J., Zhao, B., Zhang, Z., Ma, H., Sun, G., Duan, X., Duan, X., Wu, R., Dang, W., Li, J., Zhao, B., Zhang, Z., Ma, H., Sun, G., Duan, X., Tao, Q., Liu, Y., Li, B., 2019. van der Waals Epitaxial Growth of Atomically Thin 2D Metals on Dangling-Bond-Free WSe₂ and WS₂. *Adv. Funct. Mater.* 29, 1806611. <https://doi.org/10.1002/ADFM.201806611>.
- [30] Li, Z., Zheng, T., Yang, M., Sun, Y., Luo, D., Gao, W., Zheng, Z., Li, J., 2024. A Dual Mode MoTe₂/WS₂/WSe₂ Double Van der Waals Heterojunctions Phototransistor for Optical Imaging and Communication. *Adv. Opt. Mater.* 12, 2400023. <https://doi.org/10.1002/ADOM.202400023>.
- [31] Zhao, Y., Qiao, J., Yu, Z., Yu, P., Xu, K., Lau, S.P., Zhou, W., Liu, Z., Wang, X., Ji, W., 2017. High-electron-mobility and air-stable 2D layered PtSe₂ FETs. *Adv. Mater.* 29, 1604230.
- [32] Yang, X., Qin, X., Luo, J., Abbas, N., Tang, J., Li, Y., Gu, K., 2020. HfS₂/MoTe₂ vdW heterostructure: bandstructure and strain engineering based on first-principles calculation. *RSC Adv.* 10, 2615–2623.
- [33] Lee, W.-Y., Kang, M.-S., Kim, G.-S., Choi, J.W., Park, N.-W., Sim, Y., Kim, Y.-H., Seong, M.-J., Yoon, Y.-G., Saitoh, E., 2022. Interface-induced seebeck effect in PtSe₂/PtSe₂ van der Waals Homostructures. *ACS Nano* 16, 3404–3416.
- [34] Qiao, H., Zhang, Y., Yan, Z.-H., Duan, L., Fan, J.-B., Ni, L., 2022. The type-II PtSe₂/WS₂ van der Waals heterostructure: a high efficiency water-splitting photocatalyst. *Surf. Sci.* 723, 122103.
- [35] Han, S., Li, Y., Wang, Z., 2020. PtSe₂ 2/SiH van der Waals type-II heterostructure: a high efficiency photocatalyst for water splitting. *Phys. Chem. Chem. Phys.* 22, 17145–17151.
- [36] Chen, Y., Zhu, Q., Zhu, X., Sun, Y., Cheng, Z., Xu, J., Xu, M., 2023. Gate-tunable high-performance broadband phototransistor array of two-dimensional PtSe₂ on SOL. *Nano Res.* 16, 7559–7567. <https://doi.org/10.1007/S12274-022-5312-4/METRICS>.
- [37] Iqbal, M.W., Iqbal, M.Z., Khan, M.F., Shehzad, M.A., Seo, Y., Park, J.H., Hwang, C., Eom, J., 2015. High-mobility and air-stable single-layer WS₂ field-effect transistors sandwiched between chemical vapor deposition-grown hexagonal BN films. *Sci. Rep.* 5, 10699.
- [38] Fang, H., Chuang, S., Chang, T.C., Takei, K., Takahashi, T., Javey, A., 2012. High-performance single layered WSe 2 p-FETs with chemically doped contacts. *Nano Lett.* 12, 3788–3792. https://doi.org/10.1021/NL301702R/SUPPL_FILE/NL301702R_SI_001.PDF.
- [39] Si, K., Ma, J., Lu, C., Zhou, Y., He, C., Yang, D., Wang, X., Xu, X., 2020. A two-dimensional MoS₂/WSe₂ van der Waals heterostructure for enhanced photoelectric performance. *Appl. Surf. Sci.* 507, 145082.
- [40] Zheng, Y., Ma, X., Yan, F., Lin, H., Zhu, W., Ji, Y., Wang, R., Wang, K., 2022. Spin filtering effect in all-van der Waals heterostructures with WSe₂ barriers. *npj 2D Mater. Appl.* 6, 62.
- [41] Sharma, S., Singya, P.K., Deka, K., Adjih, C., Sharma, M., 2025. Terahertz communication: state-of-the-art and future directions. *IEEE Open Journal of the Communications Society* 6, 6281–6322.
- [42] Li, X., Li, J., Li, Y., Ozcan, A., Jarrahi, M., 2023. High-throughput terahertz imaging: progress and challenges. *Light Sci. Appl.* 12, 233.
- [43] Mohebbi, E., Pavoni, E., Pierantoni, L., Stipa, P., Laudadio, E., Mencarelli, D., 2024. 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. Solid.* 185, 111755.
- [44] Aytekin, Y.S., Vergnaud, C., Sharma, R., Marty, A., Pavoni, E., Mohebbi, E., Laudadio, E., Jamet, M., Mencarelli, D., Altan, H., 2026. Ultrafast carrier dynamics and electronic properties of PtSe₂/MoSe₂ and WSe₂ 2D TMDC layered structures on mica: combined THz spectroscopy and DFT study. *RSC Adv.* 16, 425–438.
- [45] Pavoni, E., Mohebbi, E., Zampa, G.M., Stipa, P., Pierantoni, L., Laudadio, E., Mencarelli, D., 2024. First principles study of WSe₂ 2 and the effect of V doping on the optical and electronic properties. *Mater. Adv.* 5 (6), 2230–2237.
- [46] Mohebbi, E., Pavoni, E., Stipa, P., Petroselli, M., Minnelli, C., Pierantoni, L., Mencarelli, D., Aldrigo, M., Laudadio, E., Fakhrabadi, M.M.S., 2025. 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*, 100947.
- [47] Mohebbi, E., Pavoni, E., Stipa, P., Petroselli, M., Pierantoni, L., Laudadio, E., Mencarelli, D., 2025. Reliable prediction of the band gap properties of graphene buffer layer on SiC using meta-GGA approximation. *Carbon Trends*, 100575.
- [48] Huang, J., Xu, N., Wu, Y., Ran, X., Fang, Y., Zhu, H., Wang, W., Chen, H., Deng, S., 2025. Interactions of Terahertz Photons with Phonons of Two-Dimensional van der Waals MoS₂/WSe₂/MoS₂ Heterostructures and Thermal Responses. *Materials* 18, 1665.
- [49] Wang, P., Wang, Y., Bian, A., Hao, S., Miao, Q., Zhang, X., He, J., He, D., Zhao, H., 2022. Energy transfer in a type-I van der Waals heterostructure of WSe₂/PtSe₂. *2D Mater.* 9, 035019.
- [50] Smidstrup, S., Markussen, T., Vancraeyveld, P., Wellendorff, J., Schneider, J., Gunst, T., Verstichel, B., Stradi, D., Khomyakov, P.A., Vej-Hansen, U.G., 2019. QuantumATK: an integrated platform of electronic and atomic-scale modelling tools. *J. Phys. Condens. Matter* 32, 015901.
- [51] Kohn, W., Sham, L.J., 1965. Self-consistent equations including exchange and correlation effects. *Phys. Rev.* 140, A1133.
- [52] Ernzerhof, M., Scuseria, G.E., 2000. Perspective on “Inhomogeneous electron gas” Hohenberg P, Kohn W (1964) *phys rev* 136: B864. *Theor. Chem. Acc.* 103, 259–262.
- [53] Sánchez-Portal, D., Ordejon, P., Artacho, E., Soler, J.M., 1997. Density-functional method for very large systems with LCAO basis sets. *Int. J. Quant. Chem.* 65, 453–461.
- [54] Mohebbi, E., Pavoni, E., Mencarelli, D., Stipa, P., Pierantoni, L., Laudadio, E., 2022. PBEsol/HSE functional: a promising candidate for vanadium dioxide (B) characterization. *RSC Adv.* 12, 31255–31263.
- [55] Heyd, J., Scuseria, G.E., 2004. Efficient hybrid density functional calculations in solids: assessment of the heyd–scuseria–ernzerhof screened coulomb hybrid functional. *J. Chem. Phys.* 121, 1187–1192.
- [56] Peter, J., Vijay, S., Choudhary, T., Biswas, R.K., 2025. Electronic bandgap prediction of functionalized MX₂-based materials using machine learning-aided and first-principles studies. *ChemistrySelect* 10, e202500536.
- [57] Rehman, S.U., Ding, Z.J., 2018. Enhanced electronic and optical properties of three TMD heterobilayers. *Phys. Chem. Chem. Phys.* 20, 16604–16614.
- [58] Ketola, T., Macháčová, N., Karlický, F., 2020. Optical gaps and excitonic properties of 2D materials by hybrid time-dependent density functional theory: evidences for monolayers and prospects for van der Waals heterostructures. *J. Chem. Theor. Comput.* 16, 5876–5883.
- [59] Zhao, Q., Guo, Y., Si, K., Ren, Z., Bai, J., Xu, X., 2017. Elastic, electronic, and dielectric properties of bulk and monolayer ZrS₂, ZrSe₂, HfS₂, HfSe₂ from van der Waals density-functional theory. *Phys. Status Solidi* 254, 1700033.
- [60] Van On, V., Nguyen, D.K., Guerrero-Sanchez, J., Hoat, D.M., 2021. Exploring the electronic band gap of janus MoSeO and WSeO monolayers and their heterostructures. *New J. Chem.* 45, 20776–20786.
- [61] Bhattacharyya, S., Singh, A.K., 2012. Semiconductor-metal transition in semiconducting bilayer sheets of transition-metal dichalcogenides. *Phys. Rev. B Condens. Matter* 86, 075454.
- [62] Ehrlich, S., Moellmann, J., Reckien, W., Bredow, T., Grimme, S., 2011. System-dependent dispersion coefficients for the DFT-D3 treatment of adsorption processes on ionic surfaces. *ChemPhysChem* 12, 3414–3420.

- [63] Desjarlais, M.P., 2005. Density functional calculations of the reflectivity of shocked xenon with ionization based gap corrections. *Contrib. Plasma Phys.* 45, 300–304.
- [64] Sipe, J.E., Ghahramani, E., 1993. Nonlinear optical response of semiconductors in the independent-particle approximation. *Phys. Rev. B* 48, 11705.
- [65] Wang, Y., Li, L., Yao, W., Song, S., Sun, J.T., Pan, J., Ren, X., Li, C., Okunishi, E., Wang, Y.Q., Wang, E., Shao, Y., Zhang, Y.Y., Yang, H.T., Schwier, E.F., Iwasawa, H., Shimada, K., Taniguchi, M., Cheng, Z., Zhou, S., Du, S., Pennycook, S. J., Pantelides, S.T., Gao, H.J., 2015. Monolayer PtSe₂, a new semiconducting transition-metal-dichalcogenide, epitaxially grown by direct selenization of Pt. *Nano Lett.* 15, 4013–4018. https://doi.org/10.1021/ACS.NANOLETT.5B00964/SUPPL_FILE/NL5B00964_SI_001.PDF.
- [66] Zhao, Y., Qiao, J., Yu, Z., Yu, P., Xu, K., Ping Lau, S., Zhou, W., Liu, Z., Wang, X., Ji, W., Chai, Y., Zhao, Y., Qiao, J., Xu, K., Lau, S.P., Chai, Y., Ji, W., Yu, Z., Wang, X., Yu, P., Liu, Z., Zhou, W., 2017. High-electron-mobility and air-stable 2D layered PtSe₂ FETs. *Adv. Mater.* 29, 1604230. <https://doi.org/10.1002/ADMA.201604230>.
- [67] Pavoni, E., Mohebbi, E., Zampa, G.M., Stipa, P., Pierantoni, L., Laudadio, E., Mencarelli, D., 2024. First principles study of WSe₂ and the effect of V doping on the optical and electronic properties. *Mater. Adv.* 5, 2230–2237. <https://doi.org/10.1039/D3MA00940H>.
- [68] Cao, B., Ye, Z., Yang, L., Gou, L., Wang, Z., 2021. Recent progress in van der Waals 2D PtSe₂. *Nanotechnology* 32, 412001.
- [69] Pezo, A., Massabeau, S., Miljević, F., Li, J., Ibrahim, F., Jamet, M., Chshiev, M., George, J.-M., Jaffrès, H., 2025. Spin and Orbital Rashba Response in Ferroelectric Polarized Ptse \$ _2 \$/MoSe \$ _2 \$/LiNbO \$ _3 \$ Heterostructures. *ArXiv Preprint ArXiv:2509.16350*.
- [70] Liu, J., Shen, T., Ren, J.-C., Li, S., Liu, W., 2023. Role of van der Waals interactions on the binding energies of 2D transition-metal dichalcogenides. *Appl. Surf. Sci.* 608, 155163.
- [71] Cappelluti, E., Roldán, R., Silva-Guillén, J.A., Ordejón, P., Guinea, F., 2013. Tight-binding model and direct-gap/indirect-gap transition in single-layer and multilayer MoS₂. *Phys. Rev. B Condens. Matter* 88, 075409.
- [72] Zeng, M., Xiao, Y., Liu, J., Yang, K., Fu, L., 2018. Exploring two-dimensional materials toward the next-generation circuits: from monomer design to assembly control. *Chem. Rev.* 118, 6236–6296.
- [73] Ju, W., Zhang, Y., Li, T., Wang, D., Zhao, E., Hu, G., Xu, Y., Li, H., 2021. A type-II WSe₂/HfSe₂ van der Waals heterostructure with adjustable electronic and optical properties. *Results Phys.* 25, 104250.
- [74] Tan, S., Dong, J., Zhao, Y., Ouyang, G., 2020. Theoretical analysis of the geometrical effects of tilted/horizontal MoS₂/WSe₂ van der Waals heterostructures: implications for photoelectric properties and energy conversion. *ACS Appl. Nano Mater.* 3, 3930–3938.
- [75] Wang, L., Jie, J., Shao, Z., Zhang, Q., Zhang, X., Wang, Y., Sun, Z., Lee, S., 2015. MoS₂/Si heterojunction with vertically standing layered structure for ultrafast, high-detectivity, self-driven visible–near infrared photodetectors. *Adv. Funct. Mater.* 25, 2910–2919.