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Two dimensional heterostructures formed by graphene-like ZnO and MgO monolayers for optoelectronic applications

Mahsa Seyedmohammadzadeh,[1] Cem Sevik,[2,3] and Oğuz Gülseren[1,4,*]

[1]*Department of Physics, Bilkent University, Ankara 06800, Turkey*
[2]*Department of Mechanical Engineering, Faculty of Engineering,*
Eskisehir Technical University, Eskisehir 26555, Turkey.
[3]*Department of Physics & NANOlab Center of Excellence,*
University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium
[4]*TÜBİTAK Research Institute for Fundamental Sciences, 41470 Gebze, Turkey*

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Two-dimensional heterostructures are an emerging class of materials for novel applications because of extensive engineering potential by tailoring intriguing properties of different layers as well as the ones arised from their interface. A systematic investigation of mechanical, electronic and optical properties of possible heterostructures formed by bilayer structures graphene-like ZnO and MgO monolayers is presented. Different functionality of each layer makes these heterostructures very appealing for device applications. ZnO layer is convenient for electron transport in these structures, while MgO layer improves electron collection. At the outset, all of the four possible stacking configurations across the heterostructure are mechanically stable. In addition, stability analysis using phonon dispersion reveals that the AB stacking formed by placing the Mg atom on top of the O atom of the ZnO layer is also dynamically stable at zero temperature. Henceforth, we have investigated the optical properties of these stable heterostructures by applying many-body perturbation theory within the framework of GW approximation and solving the Bethe-Salpeter equation. It is demonstrated that strong excitonic effects reduce the optical band gap to the visible light spectrum range. These results show that this new 2D form of ZnO/MgO heterostructures open an avenue for novel optoelectronic device applications.

I. INTRODUCTION

Following the exfoliation of single-layer graphene [1, 2], the theoretical and experimental demonstration of its many outstanding physical properties [3–7] have initiated a new nano-device engineering era. Afterwards, prediction and fabrication of other novel two-dimensional (2D) materials with different functionalities have commenced many investigations. Up to now, several various categories of 2D materials are theoretically predicted or experimentally fabricated. Examples are transitional metal dichalcogenides [8–11], MXenes [12–14], MBenes [15–17] and binary 2D structures of group II-V [18], group III–V [19] and group IV-IV [19]. Besides, 2D materials such as silicene [20, 21], h-BN [2, 22, 23] and phosphorene [24] are already explored. Most recently, Janus monolayers have attracted interest due to their distinguished properties arising from out-of-plane structural asymmetry [25–27].

Among all categories above, van der Waals heterostructures (vdWHs) formed by different monolayers are an emerging class of 2D materials [28, 29] because of enriched functionality of the structure by combining different properties of seperate monolayers. These heterostructures are good candidates for various device applications and are considered a revolutionary class of 2D structures [30] as a consequence of large number of combination possibilities for the heterostructure. Most of the initial studies of vdWHs had focused on structures formed by graphene, h-BN and TMDs. Monolayer graphene on the h-BN substrate is the first fabricated member of this class [31]. Vertical heterostructures of graphene, h-BN and MoS_2 are utilized for fabricating tunnelling diodes and transistors [32, 33]. Enhanced photocurrent generation in layered MoS_2 and WS_2 layers sandwiched between graphene layers have been reported [34, 35]. Besides, light-emitting diodes utilizing quantum wells have been designed and fabricated by combining monolayers of graphene, h-BN and TMDs [36]. Most recently, stacked 2D MoS_2 and bulk Si has been realized for designing infrared photodetector [37].

The fascinating properties of mentioned pionering structures have inspired researchers to probe other novel vdWHs, and several structures have been already explored [38–47]. The most straightforward possible structures within this category are those formed by different binary monolayers. Currently, sustainable energy-related applications of group III-VI [48] and the electronic and optical properties of group III-V [49] vdWHs are studied.

Alongside vdWHs, recent studies have reported 2D layered heterostructures with interlayer bonding [50, 51]. Examples are borophene/graphene [52] and SnP_3/GeP_3 heterostructures [53]. Besides, an *ab initio* study has demonstrated the feasibility of artificial controlling the physical properties of vdWHs by utilizing 2D donor-

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[*] gulseren@fen.bilkent.edu.tr

acceptor heterostructures to create strong bond-like interactions between layers [54]. Interlayer bonding in 2D heterostructures alters the properties of corresponding single layers, which is not so conspicuous in vdWHs [50, 55].

In this article, we presented a systematic investigation of possible heterostructures assembled by binary hexagonal monolayers of ZnO and MgO. Graphene-like ZnO and MgO have been theoretically predicted by density functional theory (DFT) based studies [18, 56]. Theoretical reports for the lattice constant of MgO and ZnO are 3.24 Å and 3.21 Å, respectively. Nonpolar monolayer of ZnO is first observed on Ag(111) [57] and later on Pd(111) [58] and Au(111) [59] surfaces. Moreover, freestanding ZnO multi- and monolayers are presently fabricated [60–63]. Distinct theoretical studies based on GW approximation have estimated a direct bandgap of 3.01 eV [64], 3.18 eV [65] and 4.87 eV [56] for monolayer ZnO, whereas the experimentally measured value are reported as 4.48 eV [66] for monolayer obtained from ZnO(0001)surface and 4 eV [62] for graphene-like ZnO. Furthermore, it is shown that ZnO(0001) surface relaxes to graphene-like ZnO and a bandgap of 4.08 eV is obtained [67] by employing the DFT+U method. The tunability of the electronic and magnetic properties of ZnO is examined by uniaxial strain [68], doping [69–71], noble metal adsorption [72] and chemical functionalization [73]. In the case of MgO, a DFT study using HSE06 functional [74] has predicted an indirect bandgap of 4.69 eV, more an indirect to direct bandgap transition by nitrogen functionalization is reported [75]. Another work using GGA-mBJ [76, 77] functional has reported a direct bandgap of 4.2 eV at Γ point. Besides, the magnetic properties of MgO have been investigated by replacing the O atom with different nonmagnetic dopants [78–80]. It was shown that B and C dopants have magnetic half-metal characteristics, N dopant creates antiferromagnetic behaviour, and F-doped monolayer is a nonmagnetic metal.

In recent years, ZnO-based vdWHs have attracted many researchers, and their applications as photocatalyst for water splitting have been investigated [81–83]. Furthermore, tunable bandgap in WSe_2/ZnO [84], stanene/ZnO [85], ZnO/PtSSe [86], MoSSe/ZnO [87], BP/ZnO [88] and ZnO/ZnX (X = S, Se, Te) [89] are already pointed out. Presently, layered structures of ZnO and MgO have been utilized in various electronic devices. ZnO/MgO dielectrics for metal-insulator-metal capacitor [90], field-effect transistor [91] and Au/MgO/ZnO metal-insulator-semiconductor ultraviolet light emitters are currently fabricated [92]. Using bilayer MgO/ZnO, a smaller leakage current and increased shunt resistance are achieved in organic photovoltaics [92]. MgO raises the short circuit current density and fill factor in such a device. A recent study is demonstrated that microspherical MgO/ZnO bilayer can enhance the stability of self-powered lead-halide perovskite photodetectors and elevate carrier transport [93]. In particular, a recent experimental study reported that internal piezoelectric polarization fields create robust confined excitions at the 2D interface of nonpolar MgZnO/ZnO heterostructures [94].

Motivated by flourishing properties of MgO/ZnO structures and theoretically predicted close lattice match between graphene-like MgO and ZnO, we have systematically investigated mechanical and optical properties of bilayer vdWHs formed by MgO and ZnO monolayers. A previous study by C. E. Ekuma *et al.* has only presented the electronic and optical properties of MgO/ZnO and MgO/ZnO/MgO heterostructures [95] in one possible stacked structure using HSE06 hybrid functional. However, up to our knowledge, there is not any report for mechanical stabilities of different possible stacking of MgO/ZnO results. In the current study, we investigated the thermodynamical, mechanical and dynamical stabilities of four possible stacking of ZnO/MgO heterostructures. Furthermore, we employed GW approximation for better description of the electronic properties of the mechanically stable heterostructures. Besides, the optical properties are determined by solving the Bethe-Salpeter equation (BSE).

II. COMPUTATIONAL DETAILS

In this work, we considered various stacked heterostructures of MgO/ZnO, which are shown in Fig. 1. In the structure named AA_{I}, the Mg atom is placed on top of the Zn atoms. In the AA_{II} structure, the O atom, which is in the same plane as the Mg atom, is placed on top of the Zn atom. Basically, this structure can be constructured from the AA_{I} by rotating the top layer by 60° through the rotation axis through the O–O bond perpendicular to the plane and then shifting it along the armchair direction, Mg moves towards the neighbour O, by a bond length. AB_{I} structure is formed by shifting the atoms of the upper plane of AA_{II} structure along armchair direction, Mg moves away from the neighbour O towards the center of hexagon of the lower layer, by a bond length. Last structure named AB_{II} is formed by shifting the atoms of the upper plane of AA_{I} structure along armchair direction, Mg moves towards the neighbour O, by a bond length.

All calculations in this study are carried out using the planewave pseudopotential method [96–99] based on density functional theory (DFT). We employed projector augmented wave-type pseudo potentials for DFT computations within the Perdew–Burke–Ernzerhof (PBE) functional [99, 100], and in order to achieve a better approximation for vdW interactions, we utilized optB86b-vdW functional [101–103]. All computational parameters have been selected after conducting careful convergence tests. For relaxing the structures, a Γ point centered $25 \times 25 \times 1$

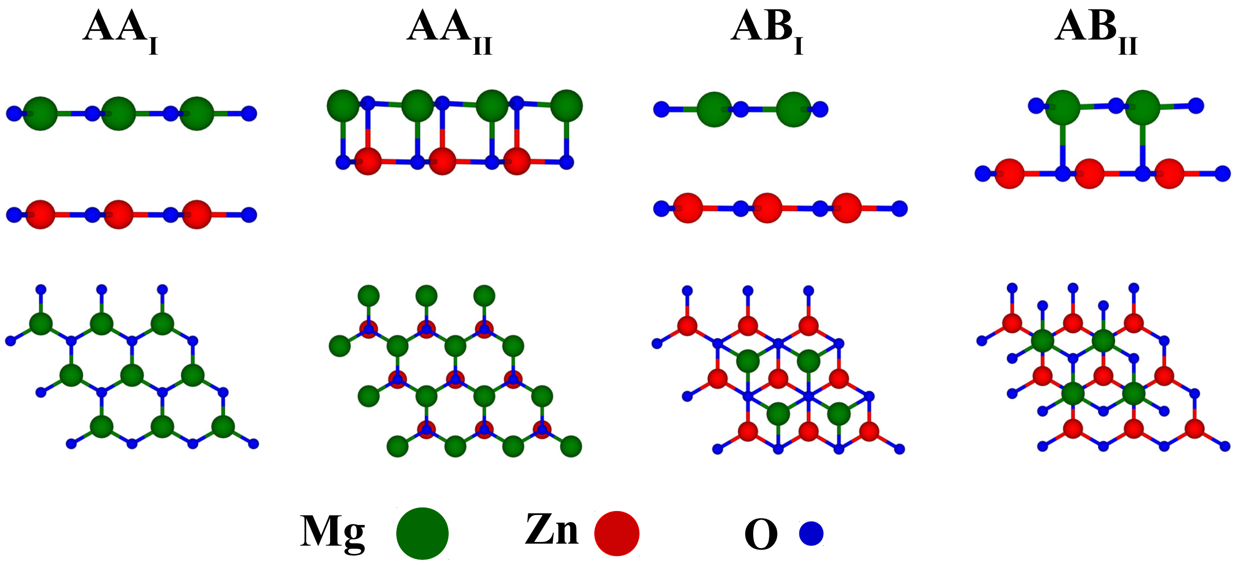

FIG. 1. Top and side views of the possible stacking of ZnO/MgO bilayer heterostructures.

Monkhorst-pack k-point mesh is used for sampling the Brillouin zone (BZ). The kinetic energy cutoff for the plane-wave basis is set to 500 eV. Energy is converged with a tolerance of 10^{-8} eV, and Hellmann–Feynman forces on each atom are minimized to be less than 10^{-3} eV/Å. In order to eliminate the interaction between the layers and their periodic images, a vacuum of 30 Å is introduced between the slabs. Subsequently, a $5 \times 5 \times 1$ supercell and $5 \times 5 \times 1$ k-point mesh are utilized for calculating phonon dispersions. Force constants are calculated using density functional perturbation theory [104], and PHONOPY [105] code is used for calculation of phonon frequencies. In order to include quasiparticle (QP) effects, we performed a single shot of GW calculation (G_0W_0). In the GW approximation, the vertex function in Hedin's equations [106] is neglected, and the self-energy (Σ) is defined as the product of the Green's function (G) and the screened Coulomb potential (W). Using DFT energies ($E_{n\mathbf{k}}$) and orbitals ($\psi_{n\mathbf{k}}$), QP energies ($E^{QP}_{n\mathbf{k}}$) in the G_0W_0 approximation are given by:

$$E^{QP}_{n\mathbf{k}} = E_{n\mathbf{k}} + Z_{n\mathbf{k}} \left\langle \psi_{n\mathbf{k}} \left| \Sigma - V_{xc} \right| \psi_{n\mathbf{k}} \right\rangle \tag{1}$$

where the indices $\mathbf{k}$ and n are crystal wave vectors and band numbers, respectively. $Z_{n\mathbf{k}}$ is the renormalization function obtained using the linearization of Σ with a series expansion around the DFT eigenvalues [107]:

$$Z_{n\mathbf{k}} = (1 - \mathrm{Re}(\frac{\partial \Sigma}{\partial \omega}\bigg|_{\omega = E_{n\mathbf{k}}}))^{-1} \tag{2}$$

In the G_0W_0 calculations, we included 800 bands (26 of them are occupied). While we use 400 eV for the kinetic energy cutoff, the number of frequency grid points is set to 160. The k-point-mesh is generated from $19 \times 19 \times 1$ grid for BZ sampling. All these parameters are selected according to convergence tests (see Fig 5 and discussions in subsection III-B).

QP energies and orbitals are used to construct self-consistent BSE [108, 109] in the Tamm-Dancoff approximation (TDA) [110–112]:

$$\begin{aligned}\left(E^{QP}_{c\mathbf{k}} - E^{QP}_{v\mathbf{k}}\right) A^{S}_{vc\mathbf{k}} \; + \sum_{v'c'\mathbf{k}'} \left\langle vc\mathbf{k} \left| K_{e-h} \right| v'c'\mathbf{k}' \right\rangle A^{S}_{v'c'\mathbf{k}'} \\ = \; \Omega^{S} A^{S}_{vc\mathbf{k}}\end{aligned} \tag{3}$$

here, indices c and v belong to conduction and valence bands, respectively, $A^{S}_{vc\mathbf{k}}$ and Ω^{S} are electron-hole coupling coefficients and corresponding BSE eigenvalues, and K_{e-h} is the kernel for electron-hole interaction. Detailed derivation and explicit form of the matrix elements of K_{e-h} can be found in reference 112 and reference 113. We considered 6 occupied bands and 12 conduction bands for solving the BSE.

III. RESULTS

A. Stability analysis

We first optimized the geometrical structures for the configurations presented in Fig. 1. Lattice parameters of the relaxed structures are given in Table I. The in-plane lattice constant of AA_I and AB_I structures are almost same, but AA_I has a slightly larger interlayer distance which is in agreement with the previously reported value [95]. The interlayer distance of these configurations is larger than their in-plane lattice constant, i.e. they are comparable with typical van der Waals bond distance. On the other hand, the obtained interlayer distances for AA_{II} and AB_{II} configurations are smaller than their in-plane lattice constants by about 1 Å. In AA_{II} and AB_{II} structures, the Mg atom is placed on top of the O atom of the underlying ZnO layer. The bond length of the Mg–O bond is 2.07 Å and 1.87 Å in its bulk form, rock salt crystal, and in monolayer MgO, respectively [18]. Hence, the calculated interlayer distances of these structures are slightly larger than of the rock salt structure. Therefore, while AA_I and AB_I structures can be considered as vdWHs, AA_{II} and AB_{II} configurations are bonded heterostructures.

We calculated the binding energies of ZnO/MgO heterostructures using the following formula:

$$E_{bind} = E_{tot} - (E_{ZnO} + E_{MgO}) \tag{4}$$

where E_{tot} is the total energy of the heterostructure, E_{ZnO} and E_{MgO} are the energy of the ZnO and MgO monolayers, respectively. The calculated binding energies are summarized in Table I. Obtained negative binding energies confirm the thermodynamic stability of all structures. The large binding energies of the AA_{II} and AB_{II} structures indicate a strong interaction between the layers.

TABLE I. Calculated in-plane lattice constant (**a**), interlayer distance (**h**), binding energy ($\mathbf{E_{bind}}$) and elastic constants ($\mathbf{C_{11}}$) and ($\mathbf{C_{12}}$) (both in $\mathbf{Nm^{-1}}$) for different stackings.

Configuration	**a (Å)**	**h (Å)**	$\mathbf{E_{bind}}$ **(meV)**	$\mathbf{C_{11}}$	$\mathbf{C_{12}}$
AA_I	3.28	3.76	-92.23	217.62	66.53
AA_{II}	3.36	2.18	-806.49	166.56	49.13
AB_I	3.28	3.53	-113.61	216.76	66.10
AB_{II}	3.32	2.36	-436.53	191.33	59.15

To further study the stability of considered materials, we computed elastic constants using the energy-strain method [114]. In terms of elastic constants C_{ij}, the criteria for mechanical stability of a 2D hexagonal lattice are given by [115, 116]:

$$\begin{aligned} C_{11} &> 0 \\ C_{11} &> |C_{12}| \end{aligned} \tag{5}$$

The pre-and post-processing steps for calculating elastic constants are carried out using the open-source program VASPKIT [117]. According to obtained results that are presented in Table I all of the configurations are mechanically stable.

To confirm the dynamical stability of the considered systems, we calculated the phonon dispersion curves as presented in Figure 2. Our results show that AB_{II} has no imaginary phonon frequency and is dynamically stable at zero temperature. AA_{II} structure possesses many imaginary frequencies, and its phonon band structure is not presented here (see supplemental material [118]). The AA_{II} structure is dropped from the analysis in the rest of the paper. AA_I and AB_I configurations have imaginary optical phonon frequencies near the center of BZ. These kinds of imaginary frequencies might be cleared by effects like temperature, strain, doping etc. An example of this kind of transition is the surface-functionalized ZnO nanostructures [73, 95]. Other examples are the bulk structures of perovskites that possess imaginary frequencies at the ground state, but temperature-dependent DFT calculations confirmed their dynamical stabilities at room temperatures [119, 120].

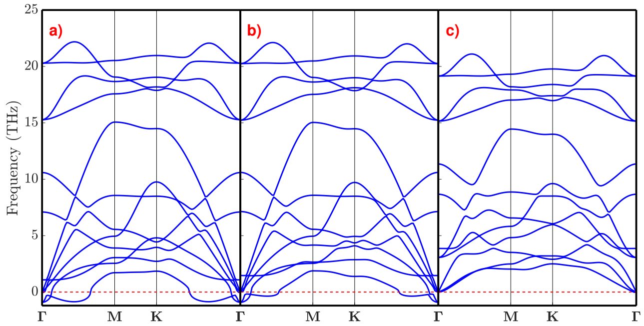

FIG. 2. Calculated phonon dispersion curves for AA_I (a), AB_I (b) and AB_{II} (c).

Apart from the stability of AB_{II}, using the obtained phonon frequencies, it is possible to compare its thermal conductivity (TC) with the monolayer ZnO approximately. A first-principle study within the framework of Boltzmann transport theory has reported a very low TC as 4.5 $Wm^{-1}K^{-1}$ for monolayer ZnO at room temperature [121]. TC of the MgO is obtained as 64 $Wm^{-1}K^{-1}$ utilizing the same procedure [122]. Here we use the Slack equation [123–125] to estimate the thermal conductivity of the AB_{II} configuration. According to the Slack equation, the thermal conductivity can be approximated by the following expression:

$$\kappa = B\frac{\bar{M}\Theta_D^3\delta n^{\frac{1}{3}}}{\gamma^2 T} \tag{6}$$

where B is a physical constant, $\bar{M}$ is the average mass of the atoms inside the primitive cell, Θ_D is the Debye temperature, δ^3 is the volume per atom, n is the number of the atoms inside the unit cell, T is the temperature, and γ is the high temperature limit of the Grüneisen parameter of acoustic modes. Using $\bar{\mathrm{M}}$ in atomic mass units and δ in Å, the constant B must be set to 3.6×10^{-6} to get κ in $\mathrm{Wm^{-1}K^{-1}}$. The Debye temperature can be approximated by following expression:

$$\frac{1}{\Theta_{\mathrm{D}}^{3}}=\frac{1}{2}\left(\frac{1}{\Theta_{\mathrm{TA}}^{3}+\Theta_{\mathrm{LA}}^{3}}\right) \tag{7}$$

The variable $\Theta_{\mathrm{i}}(\mathrm{i}=\mathrm{TA},\mathrm{LA})$, which is defined for the transverse (TA) and longitudinal (LA) acoustic modes, is given by:

$$\Theta_{\mathrm{i}}=\frac{\hbar\omega_{\mathrm{i,max}}}{\mathrm{k_B}} \tag{8}$$

where $\hbar$ is the reduced Planck constant, $\mathrm{k_B}$ is the Boltzmann constant, and $\omega_{\mathrm{i,max}}$ shows the maximum angular frequency of the LA or TA mode. The Grüneisen parameter can be chosen as 2 for all 2D materials as an approximation [125]. It is shown that this value can give a reasonably good estimation for the TC trend of 2D materials. The Debye temperature has been reported to be 287.5 K for monolayer ZnO. Using the phonon frequencies of the $\mathrm{AB_{II}}$ structure, we obtained its Debye temperature as 171.27 K. Following reference 121, here we employed the vdW diameter of the oxygen atom (3.04 Å) for the thickness of the layer. The calculated TC for ZnO and $\mathrm{AB_{II}}$ structures are 2.75 $\mathrm{Wm^{-1}K^{-1}}$ and 11.14 $\mathrm{Wm^{-1}K^{-1}}$, respectively. Despite the inaccuracy arising from the approximations, this result shows that the $\mathrm{AB_{II}}$ structure has a smaller TC than monolayer ZnO and MgO.

B. Electronic properties

Next, we investigated the electronic structure of ZnO/MgO heterostructures. The DFT band structures are shown in Fig. 3, and the bandgap values are summarized in Table II. $\mathrm{AA_I}$ and $\mathrm{AB_I}$ structures exhibit direct band gaps transition at the Γ point, but $\mathrm{AB_{II}}$ has an indirect bandgap. Compared to the ZnO and MgO monolayers, the location of maximum of the valence band (VBM) and the minimum of the conduction band (CBM) of the structures indexed by I and II are the same as the ZnO and MgO monolayers, respectively. The DFT bandgap of the $\mathrm{AA_I}$ is 1.58 eV, which is larger than of $\mathrm{AB_I}$ structure by a small amount of 0.01 eV. The indirect bandgap of $\mathrm{AB_{II}}$ is 1.87 eV. This different characteristic of the band gap is another result of the bonded inter-layer nature of the heterostructure. For this structure, the minimum bandgap for a direct transition which is essential in our BSE calculation is located at the Γ point and has a value of 2.13 eV. The LDA bandgaps for ZnO and MgO have been reported as 1.68 eV and 3.68 eV, respectively [18]. In comparison to the large bandgap of MgO, the band gaps of the considered heterostructures are decreased by 57.07% in the case of $\mathrm{AA_I}$, 57.33% in $\mathrm{AB_I}$ and 49.20% in $\mathrm{AB_{II}}$. The DFT bandgap of the $\mathrm{AB_{II}}$ structure is 0.19 eV larger than the ZnO monolayer.

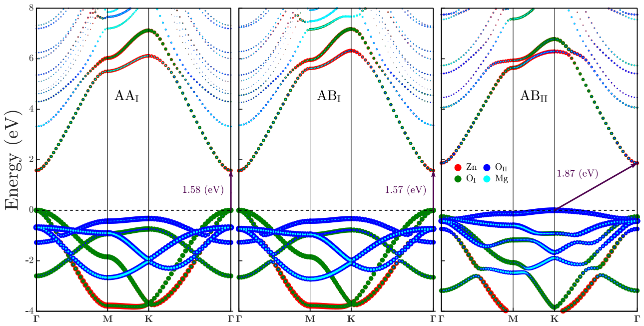

FIG. 3. Electronic band structures of $\mathrm{AA_I}$, $\mathrm{AB_I}$ and $\mathrm{AB_{II}}$. The band energies are shifted so that the maximum of the valence band is located at E=0 eV. The arrows show the band gap.

TABLE II. Calculated DFT bandgap ($\mathbf{E_{vdW}}$), $\mathrm{G_0W_0}$ bandgap ($\mathbf{E_{G_0W_0}}$), first BSE eigenvalue ($\mathbf{E_{BSE}}$) and exciton binding energies ($\mathbf{E_{exc}}$). All energies are in eV. The direct band gap of the $\mathrm{AB_{II}}$ structure (4.42 eV) is used for calculation of the exciton binding energy.

Configuration	$\mathbf{E_{vdW}}$	$\mathbf{E_{G_0W_0}}$	$\mathbf{E_{BSE}}$	$\mathbf{E_{exc}}$
$\mathrm{AA_I}$	1.58	3.73	2.50	1.23
$\mathrm{AB_I}$	1.57	3.70	2.49	1.21
$\mathrm{AB_{II}}$	1.87	4.07	3.05	1.37

The contribution of each atom in the band structure is also displayed in Fig. 3. Furthermore, we presented the total density of states (DOS) and orbital decomposed DOS for each atom in mechanically stable structures in Fig. 4. Inspection of Fig. 4 shows that the top of the valence band is dominated by the orbitals from the MgO layer in the $\mathrm{AB_{II}}$ structure. In the systems labeled by I, the orbitals of the atoms in the ZnO layer form the top of the valence band. In all structures, Zn atom has the most contribution in the first conduction band. These results show that the MgO layer enriches the electron collection in the bonded bilayer, and the ZnO layer acts as an electron transfer layer.

After this detailed discussion of the band structure, we can identify the band alignment across the heterostructure. The band alignment of these vertical heterostructures, i.e. the bilayer structures formed by different layers A and B, can be determined according to the position of VBM and CBM of the different layers [126]. In straddling (type-I) heterostructures $\mathrm{VBM_A} < \mathrm{VBM_B} < \mathrm{CBM_B} < \mathrm{CBM_A}$, hence, electrons and holes are confined in the same region, which can lead to radiative recombinations. Hence, type-I alignment

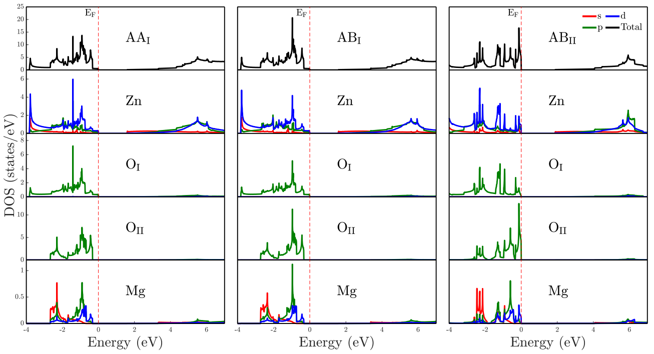

FIG. 4. Total and partial density states of AA_I, AB_I and AB_{II} structures. O_I and O_{II} are the oxygen atoms in the same layer with Zn and Mg atoms, respectively.

is desirable for applications such as light emitting diodes (LEDs). In staggered (type-II) heterostructures, $VBM_A < VBM_B < CBM_A < CBM_B$, therefore VBM and CMB of the type-II heterostructures are placed in different layers that facilitates separation of electrons and holes. Type-II heterostructures are promising for applications such as photovoltaics, photo-detection, solar cells and lasers. In our cases, as we have stated before from band structures, Zn atom has the most contribution in the first conduction band, while the orbitals of the atoms in the ZnO and MgO layers, for structures labeled by I and II respectively, form the top of the valence band. Therefore, AA_I and AB_I heterostructures exhibit type-I band alignment, with $VBM_{MgO} < VBM_{ZnO} < CBM_{ZnO} < CBM_{MgO}$. The band alignment of the AA_I structure is predicted as type-I alignment [95] which is consistent with this result. On the other hand, AB_{II}, $VBM_{ZnO} < VBM_{MgO} < CBM_{ZnO} < CBM_{MgO}$ that indicates type-II band alignment.

We calculated Bader's charges associated with each atom in order to further understand the bonding nature between the atoms. For Bader analysis, the charge attributed to each atom is calculated using the minima of the charge density between the atoms [127–129]. The obtained Bader charges are summarized in Table III. The Bader charges are reported as charge transfer on each atom with respect to their atomic configurations. Therefore, negative charge means electron excess while the positive charge means deficiency. The Bader charges of the structures labeled by I indicate that, approximately, 1.19e is donated by Zn atom to the O atom in the same layer, which received 1.2e in total. The charge transfer is slightly larger in MgO layer, 1.64e of Mg is transfer to O in the same layer, receiving 1.63e in total. Hence, there is only 0.01e transfer from MgO layer to ZnO in these structures, which also verifies their van der Waals character. On the other hand, we observed a more mixed situation in AB_{II} structure. Still, Zn donates 1.19e and Mg gives away 1.64e similar to the vdWHs, approximately. However, the O of ZnO layer receives 1.24e while the MgO layer O only draws 1.59e. Therefore, the charge transfer from MgO layer to ZnO is slightly larger and increases to 0.04e. This can be interpreted by comparing the bond length of AB_{II} configuration with other structures. According to the lattice constant values summarized in Table I, AB_{II} has a smaller inter-layer separation and metal atoms approach to the inter-layer O atoms. The calculated negative Bader charge for the O_I atom in the AB_{II} structure is 0.043e smaller than the O_I atom in other structures, which shows the interaction between the Mg atom of the AB_{II} structure and the O_I atom, this is consistent with the smaller interlayer distance of the AB_{II} structure. These results show a stronger interaction between the layers in AB_{II} structure consistent with bonded inter-layer nature of the heterostructure.

TABLE III. Calculated Bader charges for each atom in different configurations. $\mathbf{O_I}$ and O_{II} are the atoms on ZnO and MgO layers, respectively.

Configuration	**Zn**	**O_I**	**O_{II}**	**Mg**
AA_I	1.191	-1.199	-1.628	1.636
AB_I	1.187	-1.199	-1.625	1.637
AB_{II}	1.186	-1.242	-1.586	1.642

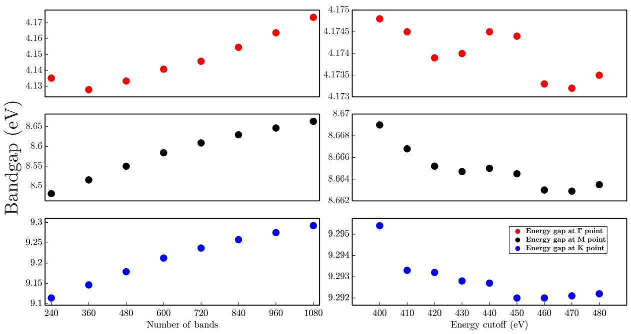

FIG. 5. Examples of quasiparticle energy convergence tests for AB_I structure with respect to number of bands (left) and energy cutoff (right). For the convergence test of the number of bands, the energy cutoff has been set to 480 eV. For the energy cutoff, 1080 bands are used. In both cases, the number of (imaginary) frequency grid points is chosen as 200, and a vacuum of 30 Å is considered.

Up to now, we have outlined standard electronic properties of the considered structures at the DFT level. At this point, we turn our attention to excited states and excitonic effects for optical properties. First of all, we used G_0W_0 approach for the treatment of the quasiparticle effects. There are several parameters that can affect the accuracy of the GW-BSE method.

First, the number of (imaginary) frequency grid points is chosen as 160 for all cases. Two main factors are the number of unoccupied bands and the energy cutoff for the response function. Furthermore, in the case of the 2D structures, the amount of the vacuum distance considered above the slab is critical because of the long range nature of Columb interaction. The other important factor is the k-point mesh used for BZ sampling. Fully converged results can only be achieved using a very dense k-point mesh [130], i.e. up to 300 × 300 × 1. However, the excessive memory requirements prevent using very dense k-point mesh and a large vacuum distance above the slab. After emphasizing these points, we selected 19 × 19 × 1 k-point mesh and a vacuum of 30 Å for all structures, considering the results of references 131–133. We used 6 × 6 × 1 to estimate the number of the required empty bands and energy cutoff for the response function to minimize the error in the G_0W_0 bandgap up to 0.1 eV. An example of convergence tests is presented in Fig. 5. The G_0W_0 bandgap is very sensitive to the number of empty bands, but the energy cutoff value has a negligible effect on the bandgap of the materials considered in this study. We selected 800 empty bands and an energy cutoff of 400 eV for plane-wave energy, while 2/3 of this value is used for the energy cutoff for the response function. Parameters similar to those selected here were previously used to derive scaling universality between band gap and exciton binding energy of 2D materials [132, 133].

It is commendable to note that utilizing the wave functions from the DFT+U or HSE methods can improve the convergence of the GW calculation for materials with d orbital shells. However, the HSE method imposes a high computational cost, and parameterizing DFT+U is challenging without prior experimental knowledge. In the specific case of the considered 2D materials for assembling the heterostructures considered in this study, it must be pointed out that in the MgO structure, the Mg atom has a full s orbital shell, and correlation effects are not significant in this material. It is evident from the slight difference in the predicted band gap of g-MgO using DFT and HSE [18]. Besides, a good agreement with experimental measurements has been obtained using well converged GW method using KS orbitals [134]. On the other hand, possessing a closed d orbital shell, ZnO must be treated carefully. Determining the structural and electronic properties of bulk ZnO using DFT+U has been considered in several studies. For monolayer ZnO, the band gap from HSE is calculated 50% larger compared to the DFT one [18]. Recently, the effect of Hubbard U correction on the band gap of monolayer ZnO is investigated in detail [135], and it is pointed out that further experimental data is required for the correct selection of the DFT+U parameters. Here, it is worthy to emphasize that GW_0+U_d improves the calculated band gap of bulk ZnO by considering 160 bands for the band summation [136]. Similarly, it is shown that by increasing the number of unoccupied bands considered in the G_0W_0 calculation, the band gap converges to the experimental value, but LDA+U+G_0W_0 converges more rapidly than the LDA+G_0W_0 [137]. Furthermore, a similar effect is reported in the case of transition metal oxide perovskites, and the effect of converged number of bands in the results of GW calculations is highlighted [138]. Therefore, although we emphasize the importance of the considered initial orbitals in GW calculations, we rely on DFT orbitals and careful convergence tests performed for selecting the parameters in this study.

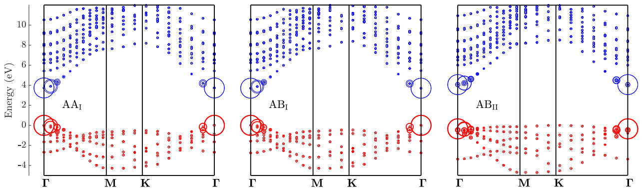

FIG. 6. The band structure calculated by G_0W_0 approach. The circles show the absolute value of the coupling coefficients. The radii of the circles are scaled according to the maximum coupling coefficient and the gap between the band structure.

First, the band structures calculated within G_0W_0 approach are displayed in Fig. 6. Comparison of these with the band structures calculated within the standard DFT approach (see Fig. 3) show that mostly the band gaps increase without much change in band dispersion because of quasiparticle interactions. The obtained bandgaps from G_0W_0 calculations, ($E_{G_0W_0}$), are presented in Table II. The quasiparticle effects increase the bandgaps more than 50%. In all configurations, the calculated $E_{G_0W_0}$ is risen more than twice to the IR region of the spectrum. These relative factors show the similar nature of the electron-hole interaction in different considered systems. As previously pointed out, the results of the GW-BSE method are sensitive to the used computational parameters. Therefore, it is necessary to be careful for an exact quantitative compression between the results obtained in this work and previous literature reports. The G_0W_0 bandgap of monolayer ZnO has been reported to be 4.87 eV [56], 3.18 eV [65], 3.01 eV [64], and 3.98 eV [139]. Compared with the experimentally reported bandgap value of 4.00 eV for graphene-like ZnO [62], the calculated G_0W_0 bandgaps of the AA_I and AB_I are smaller by 0.27 eV 0.3 eV, respectively. AB_{II} possesses a broader bandgap by 0.07 eV.

The first BSE eigenvalues, E_{BSE}, which are used for the calculation of exciton binding energy, (E_{exc}), are also reported in Table II. E_{exc} is just the difference between the first BSE eigenvalue and the corresponding G_0W_0 direct bandgap (see Table II). The first bright exciton of the AB_{II} structure has a binding energy (E_{exc}) of 1.37 eV, which is the maximum among all configurations. The excitonic eigenstates can be expressed by the sum of eigenstates of the electron-hole pairs:

$$|\mathrm{S}\rangle = \sum_{vc\mathbf{k}} A^{S}_{vc\mathbf{k}} \, |vc\mathbf{k}\rangle \tag{9}$$

According to equation 9, visualizing coupling coefficients can give information about the electron-hole pairs that contribute more to the specific exciton wave function, denoted by $|\mathrm{S}\rangle$. So, the absolute value of BSE coupling coefficients are shown in fatband representation [140] along with the $\mathrm{G_0W_0}$ band structure in Fig. 6. Apparently, the couplings are strong near the Γ point where the direct bandgap is located. In the structures labeled by **I**, only two valence bands from the edge of the valence band (bands number 13 and 12), have large coupling values. In the $\mathrm{AB_{II}}$ stacking, notable couplings are also observable for the third valence band from the edge (11'th band).

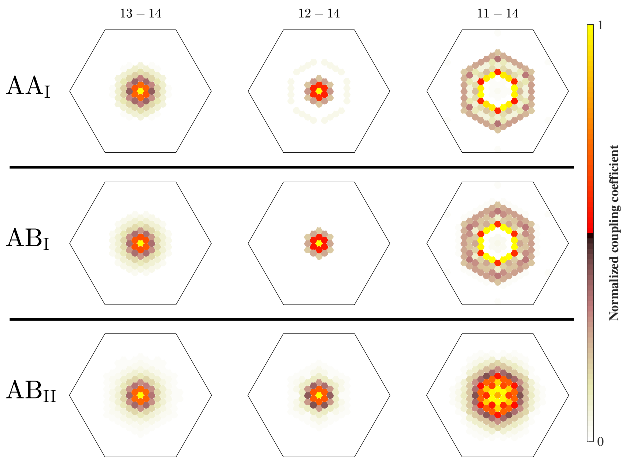

FIG. 7. Distribution of absolute value of electron-hole coupling coefficients for direct transitions from top three valence bands from the edge (bands number 13, 12 and 11) to first conduction band (band number 14). Hexagons show the first Brillouin zone.

In Fig 7, we plotted the absolute values of normalized coupling coefficients between the first conduction band (band number 14) and top three valence bands from the edge in the first BZ. The maximum coupling between the two top valence bands and the first conduction band is located at the Γ point in all structures. The coupling coefficients between the second VB and first CB band vanish more rapidly than those of VBM and CBM (bands 13-14). For $\mathrm{AA_I}$ and $\mathrm{AB_I}$, couplings are negligible near the Γ point and edges of the BZ. In $\mathrm{AB_{II}}$, the couplings have considerable values near the Γ point. These behaviours are directly related to the shape of the band structure. For example, in $\mathrm{AB_I}$ and $\mathrm{AA_I}$, the minimum distance between the third VB and first CB is located where the maximum coupling coefficient is observed.

C. Optical properties

Next, the optical properties of ZnO/MgO heterostructures will be discussed. The first BSE eigenvalues are listed in Table II. According to these results, the optical band gaps are 2.50 eV, 2.49 eV and 3.05 eV for $\mathrm{AA_I}$ and $\mathrm{AB_I}$ and $\mathrm{AB_{II}}$, respectively. The imaginary part of the dielectric functions ($\mathrm{Im}(\epsilon_{\mathrm{x}})$ for x-polarized incident light are presented in Fig. 8. The dielectric function of $\mathrm{AA_I}$ and $\mathrm{AB_I}$ structures, i.e. vdWHs, have very similar shapes. In these two structures, the blue shifts due to quasiparticle effects are reduced by 42.79% and 43.19%. Consequently, the first peaks of the dielectric functions have appeared in the middle of the visible spectrum. Besides, the dielectric functions have a shoulder near the outer edge of the violet light. For x-polarized light, the quasiparticle blue shift in the $\mathrm{AB_{II}}$ system is reduced by 46.27%, and the peak of the $\mathrm{Im}(\epsilon_{\mathrm{x}}$ is located at the inner edge of the violet light. Similar to other structures, $\mathrm{Im}(\epsilon_{\mathrm{x}}$ of $\mathrm{AB_{II}}$ also has a shoulder near the first peak, which is located at the outer edge of the violet light spectrum. Calculated optical spectra at the RPA level show that the position of the first peak in the out-of-plane dielectric function of $\mathrm{AB_{II}}$ is located (0.48 eV) after the direct band gap (4.42 eV). This distance is much more considerable in $\mathrm{AB_I}$ (1.81 eV) and $\mathrm{AA_I}$ (1.73 eV). This different behavior might be due to the different nature of the band gap, which is indirect in $\mathrm{AB_{II}}$ structure.

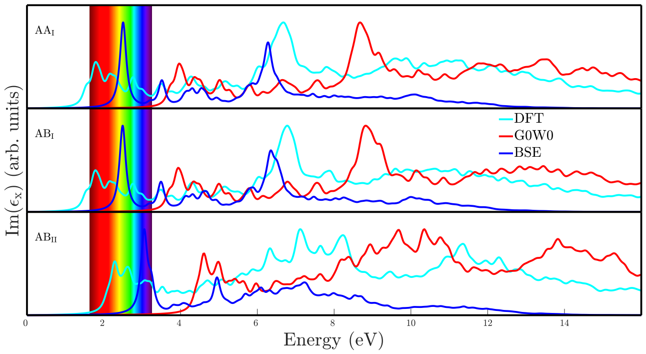

FIG. 8. The imaginary part of the dielectric function for x-polarized incident light for $\mathrm{AA_I}$ and $\mathrm{AB_I}$ and $\mathrm{AB_{II}}$ configurations. Cyan, red and blue curves are the results of the DFT, $\mathrm{G_0W_0}$ and BSE calculations. The visible light spectrum is also shown (from 1.63 eV to 3.26 eV) for reference.

In order to gain further insight into excitonic properties, we plotted oscillator strengths along with the imaginary part of the dielectric function corresponding to x-polarized and z-polarized lights as well as the optical absorbance for perpendicular incident light from BSE calculation in Fig. 9. For 2D materials, the amount of incident light that the layer can absorb is quantified by optical absorbance ($\mathrm{A}\,(\omega)$), which can be calculated by

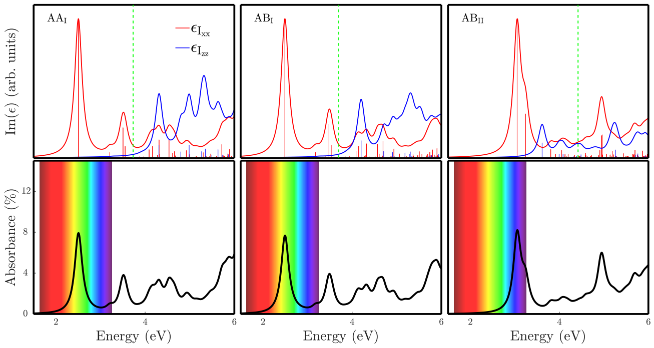

FIG. 9. (Upper row) The imaginary part of the dielectric function for x- and z-polarized incident lights from BSE calculation. Vertical blue and red lines show the oscillator strengths for x- and z-polarized, respectively. Dashed green lines show the position of direct G_0W_0 band gap. (Bottom row) Optical aborbance for perpendicular incident light from BSE calculation.

$A(\omega) = \frac{\omega}{c} L\text{Im}(\epsilon(\omega))$ as described in detail before [141], where c is the speed of light and L is the slab thickness. Despite their small thickness, some 2D materials can absorb considerable incident light. For example, graphene displays an absorbance of 2.3% in the visible light range, equivalent to 20 nm thick Si or 5 nm thick GaAs. Besides, monolayer TMDs such as MoS_2,$MoSe_2$ and WS_2 can absorb up to 5–10% of sunlight. The optical absorbance of the considered structures for the perpendicular incident light is presented in Fig 9. All structures possess a single absorbance peak at the optical band gap, and exhibit optical absorbance values similar to other 2D materials like graphene and TMDs.

The details of optical transitions can be described in terms of oscillator strengths which represent the intensity of the transition for specific excitonic states and are proportional to the sum of the momentum matrix elements [142, 143]. In all of the considered structures, the most considerable oscillator strength appeared at the energy where the first maximum of the Im(ϵ_x) is located. As it is expected, the subsequent non-zero oscillator strengths are precisely in accordance with the peaks and shoulders of the dielectric function. In all of the configurations, the first peak of the Im(ϵ_x) precedes the first peak of the Im(ϵ_z). In the AA$_I$ and AB$_I$ structures, the first peak of the Im(ϵ_z) is located after the second peak of Im(ϵ_x). In the AB$_{II}$ structure, the first peak of the Im(ϵ_z) is located close to the visible light spectrum and appears before the second peak of the Im(ϵ_x). By comparing the magnitude of the oscillator strengths, it is also possible to distinguish the dark and bright excitons. The dark excitons are those with zero or negligible oscillator strengths (see Figure 10). Dark excitons with zero oscillator strengths are related to the spin or momentum forbidden transitions [144, 145]. Since the effects of spin polarization and finite momentum are not considered in our approach, the dark excitons in Fig. 10 are related to small transition probabilities. Close energy between the dark and bright excitons can affect the photoluminescence of the nanostructures [146, 147]. Our results show that there is not any dark exciton close to the first BSE eigenvalue of the AA$_I$ and AB$_I$ structures. The first dark exciton of AB$_{II}$ structure appears near the third BSE eigenvalues.

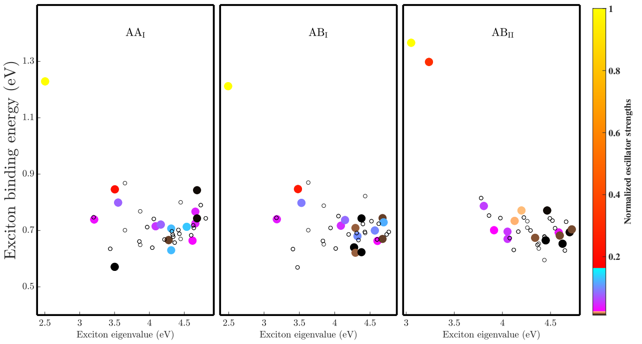

FIG. 10. The exciton binding energies versus exciton eigenvalues for x-polarized incident light. The color bar shows the normalized oscillator strengths and open black circles are used for displaying zero oscillator strengths.

IV. CONCLUSION

In summary, we studied the mechanical, electronic and optical properties of four possible heterostructures formed from ZnO and MgO monolayers. The interlayer distances show that AA$_I$ and AB$_I$ can be considered as vdWH bilayers, however there is an interlayer bonding in AB$_{II}$ and AA$_{II}$ heterostructures. These results are confirmed by comparing the amount of charge transfer between the layers. AA$_{II}$ has many imaginary frequencies in the entire BZ and is dynamically unstable. The AA$_I$ and AB$_I$ have small imaginary phonon frequencies near the center of the BZ. The AB$_I$ structure is dynamically stable at zero temperature. Our band structure calculations based on DFT show that the orbitals of Zn atom dominate the first conduction band of these structures. The MgO layer orbitals dominate the top valence band of the AB$_{II}$ structure. Henceforth, ZnO layer is convenient for electron transport in these structures, while MgO layer improves electron collection. Applying GW-BSE calculations shows strong excitonic effects in MgO/ZnO heterostructures. Our results show that the optical bandgaps of these structures are in the visible light spectrum. These results show that this new 2D form of ZnO/MgO heterostructures open an avenue for novel optoelectronic device applications.

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