Electronic Supplementary Information (ESI)

Electronic and optical properties of blue phosphorus/boron phosphide heterostructure

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I. PHONON SPECTRUM

The calculation of phonon spectrum is a reliable tool to ensure the dynamical stability of the structure. Phonon spectrum of structures are presented in Figure 1 along the high-symmetry direction in the first Brillouin zone. It is well-known fact that, spectrum consists of six phonon branches due to the D_{6h} point-group symmetry of hexagonal 2D structure, i.e., MBOP and MBP. By increasing the number of layer, number of branch become twelve and eighteen for AA (AB) and ABA (ABB and ABC), respectively. It is clear from the Figure 1 that, all branches over the first BZ have positive phonon frequencies which undertake the dynamical stability of structures. It is also obvious that phonon spectrum of MBOP is compatible with those who have found in Refs. 1 and 2

II. TIGHT-BINDING PARAMETERS

For the TB calculations we followed both single and multi-orbital models. The single orbital model includes only the on-site energy and the overlap between p_z atomic orbitals of boron and phosphor atoms. For the multi-orbital TB calculations we consider four orthogonal atomic orbitals per each B and P atom in the unit cell. After hybridization we consider three σ and one π orbitals. The on-site energy of atomic orbital were used for new hybrid orbitals and the hopping integral between orbitals are determined based on the Slater-Koster approach [3, 4]. The model includes parameters for the on-site energy of s and p atomic orbitals of B and P atoms. The hopping between neighbor atoms are defined based on four TB parameters $t_{ss\sigma}$, $t_{sp\sigma}$ $t_{pp\sigma}$ and $t_{pp\pi}$.

TABLE I: TB hopping integrals between atomic orbitals for AA and AB stacking.

Parameter	$t_{ss\sigma}$	$t_{sp\sigma}$	$t_{pp\sigma}$	$t_{pp\pi}$
MBOP	-3.15	3.25	3.2000	-1.54
P(MBOP)-P(MBP) (AA_NN)	-0.07	-0.12	-0.42	0.11
B(MBOP)-P(MBP) (AA_NN)	-0.18	0.28	-1.21	0.24
B(MBOP)-P(MBP) (AB_NN)	-0.03	0.02	0.54	-0.18
P(MBOP)-P(MBP) (AB_NNN)	0.00	0.00	0.05	-0.06

TABLE II: The on-site energy of s and p atomic orbitals for B and P atoms

Parameter	Es-B	Ep-B	Es-P	Ep-P
Value (eV)	-2.3	0.75	-6.1	-0.16

The on-site energies of s and p orbital for B and P are listed in table II.

For the AB, ABA, ABB and ABC configurations the p orbital on-site energy of P atoms reduces by 0.18 eV to reach a better agreement with DFT-PBE results. For the single-band TB model of MBOP we define two parameters, $E_{B,P}$ and t_{B-P} that are the on-site energies and hopping integrals between B and P atoms, respectively. The t_{B-P} is set to the hopping between p atomic orbitals of B and P $t_{pp\pi}$=-1.54 eV and the on-site energies for the single-orbital model are collected in table III.

The TB parameters of interaction between MBP layers in the trilayer stacking are adopted from our previous work on bilayer blue phosphorus [5]. Actually the hopping between neighbor layers are consider half of the

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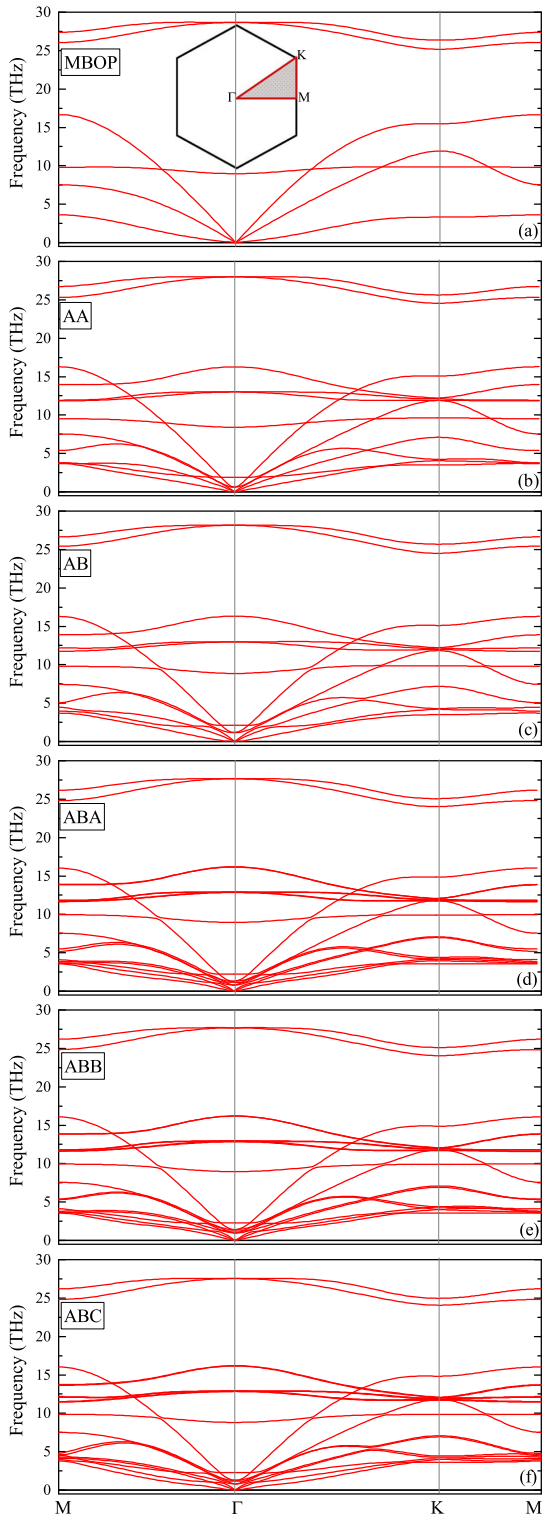

FIG. 1: Phonon spectrum of MBOP, AA, AB, and ABA.

bilayer blue phosphorus in AB stacking. For the trilayer atomic configurations, the single-orbital TB model can not address the direct-indirect band gap transition and is not presented here.

TABLE III: On-site energies of B and P atoms in the single-orbital TB model

Configuration	E_B	E_P
MBOP	0.75	-0.16
AA	0.93	-0.06
AB	0.70	-0.37

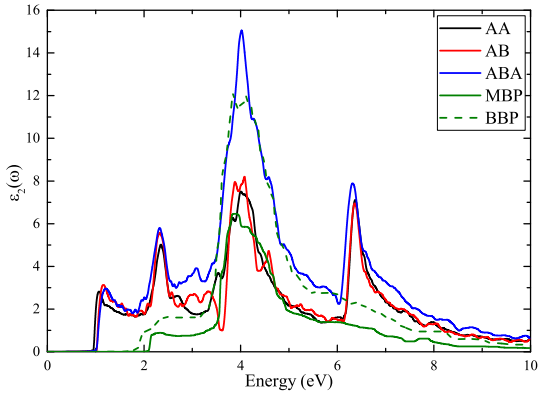

FIG. 2: (Color online) Frequency dependent imaginary dielectric function of AA, AB, ABA, MBP and BBP.

III. OPTICAL PROPERTIES

To gain a better understanding, imaginary part of frequency dependent dielectric function is also calculated for MBP and BBP in Figure 2 which was presented before in Ref.5. Aside from onset, first and last peaks, the main absorption peak of MBP and BBP are comparable with heterostructures. For the bilayer structures (AA and AB), related peak shows resemblance with the main absorption peak of MBP as peak order and broadening. A similar case is also valid between ABA (Due to similar trend of the other stacking, i.e., ABB and ABC, only ABA is presented) and BBP which supports the idea of this study. Imaginary part of frequency dependent dielectric function is also calculated for MBOP at DFT-HSE level as presented in Figure 3. Even curve has common trend, its absorption onset and and peaks yield blue shift around $\sim$ 0.5 eV which is also expected from the correction of band gap by hybrid functional (See Table I). Similar results and discussions are also presented in Refs. 6 and 7 for some 2D structures at the calculation of optical properties in the scheme of DFT-HSE.

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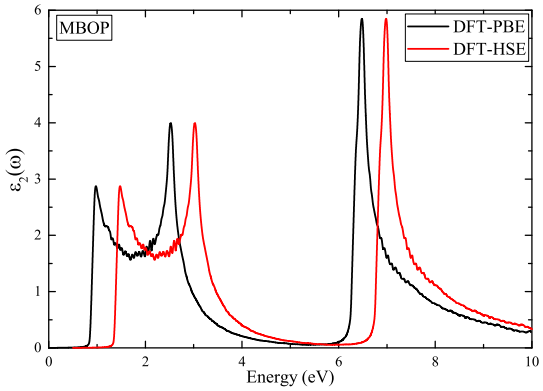

FIG. 3: (Color online) Frequency dependent imaginary dielectric function of MBOP for DFT-PBE and DFT-HSE.

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