Band offsets in new BN/BX (X = P, As, Sb) lateral heterostructures based on bond-orbital theory

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TABLE SI. Bond length, lattice constant, VBM, and CBM values of BN and BX (X = P, As, Sb) monolayers.

<table>
<thead>
<tr>
<th>Material</th>
<th>Bond Lengths (Å)</th>
<th>Lattice Constants (Å)</th>
<th>VBM (eV)</th>
<th>CBM (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>PBE</td>
<td>HSE</td>
</tr>
<tr>
<td>BN</td>
<td>1.45</td>
<td>2.51</td>
<td>-5.80</td>
<td>-6.56</td>
</tr>
<tr>
<td>BP</td>
<td>1.85</td>
<td>3.21</td>
<td>-5.08</td>
<td>-5.43</td>
</tr>
<tr>
<td>BAs</td>
<td>1.96</td>
<td>3.39</td>
<td>-4.89</td>
<td>-5.21</td>
</tr>
<tr>
<td>BSb</td>
<td>2.15</td>
<td>3.73</td>
<td>-4.49</td>
<td>-4.83</td>
</tr>
</tbody>
</table>
**TABLE SII.** Bond length and lattice constant of \((\text{BN})_n(\text{BX})_n\) \((X = \text{P, As, Sb}; n = 2, 4, 6, 8)\) lateral heterojunctions.

<table>
<thead>
<tr>
<th>LHS (Zigzag)</th>
<th>Bond Lengths (Å)</th>
<th>Lattice Constants (Å)</th>
<th>LHS (Armchair)</th>
<th>Bond Lengths (Å)</th>
<th>Lattice Constants (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>B-N</td>
<td>B-X</td>
<td></td>
<td>B-N</td>
<td>B-X</td>
</tr>
<tr>
<td>((\text{BN})_2(\text{BP})_2)</td>
<td>1.527</td>
<td>1.800</td>
<td>2.830</td>
<td>((\text{BN})_2(\text{BP})_2)</td>
<td>1.482</td>
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<tr>
<td>((\text{BN})_4(\text{BP})_4)</td>
<td>1.529</td>
<td>1.793</td>
<td>2.841</td>
<td>((\text{BN})_4(\text{BP})_4)</td>
<td>1.506</td>
</tr>
<tr>
<td>((\text{BN})_6(\text{BP})_6)</td>
<td>1.530</td>
<td>1.791</td>
<td>2.841</td>
<td>((\text{BN})_6(\text{BP})_6)</td>
<td>1.514</td>
</tr>
<tr>
<td>((\text{BN})_8(\text{BP})_8)</td>
<td>1.531</td>
<td>1.789</td>
<td>2.842</td>
<td>((\text{BN})_8(\text{BP})_8)</td>
<td>1.518</td>
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<td>((\text{BN})_2(\text{BAs})_2)</td>
<td>1.549</td>
<td>1.891</td>
<td>2.923</td>
<td>((\text{BN})_2(\text{BAs})_2)</td>
<td>1.488</td>
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<tr>
<td>((\text{BN})_2(\text{BSb})_2)</td>
<td>1.574</td>
<td>2.087</td>
<td>3.020</td>
<td>((\text{BN})_2(\text{BSb})_2)</td>
<td>1.503</td>
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</tbody>
</table>
**Fig. S1** Deformation charge density of $(\text{BN})_n(\text{BX})_n$ LHS $(n = 4, 6, 8)$ along zigzag (a) and armchair (b) directions, respectively. White and black color refer to electron accumulation and depletion region, respectively.
Fig. S2 Electron localization functions (ELFs) of the B-N and B-X bonds in \((\text{BN})_2(\text{BX})_2\) LHS.
Fig. S3 Electron localization functions (ELFs) of the B-N and B-P bonds in (BN)$_n$(BP)$_n$ LHS ($n = 4, 6, 8$).
Fig. S4 Formation energy of $\text{(BN)}_n\text{(BX)}_n$ LHS ($X = \text{P, As, Sb}; n = 2, 4, 6, 8$).
Fig. S5 (a) Calculated phonon dispersion spectra of the armchair (BN)$_2$(BP)$_2$ LHS. (b) Top (left panel) and side (right panel) views of the snapshots from the molecules dynamic simulation of atomic structures for the armchair (BN)$_2$(BP)$_2$ LHS at the temperature of 300 K.
Fig. S6 Iso-surfaces of partial charge densities for the VBM and CBM of zigzag (a) and armchair (b) (BN)$_2$(BX)$_2$ LHS.
Fig. S7 Iso-surfaces of partial charge densities for the VBM and CBM of zigzag (a) and armchair (b) (BN)$_n$(BP)$_n$ LHS ($n = 4, 6, 8$).