Electronic Supplementary Material (ESI) for Nanoscale.

Novel Antimonene Tunneling Field Effect Transistors Using an Abrupt Transition from Semiconductor to Metal in Monolayer and Multilayer Antimonene Heterostructures

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Table S1. Effective masses of electrons and holes in the armchair and zirgag directions for monolayer antimonene.

Band	CB			VB	
Valley	**Valley 1**	**Valley 2**	**Valley 3**	**Heavy Hole**	**Light Hole**
Armchair	0.472	0.175	0.175	0.432	0.079
Zigzag	0.145	0.303	0.303	0.412	0.081

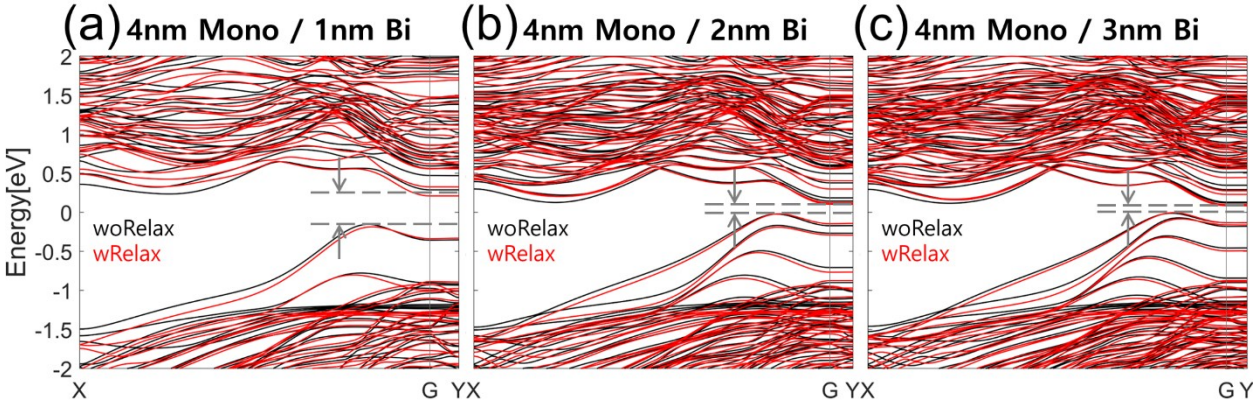

Figure S1. Band structures of monolayer/bilayer/monolayer heterostructures with different multilayer lengths L_{Multi} = (a) 1, (b) 2 and (c) 3 nm. Non-zero band gaps are denoted by arrows.

Figure S1 shows band structures of monolayer/bilayer/monolayer heterostructures for 1, 2 and 3 nm bilayer lengths, respectively. We construct heterostructures combining monolayer and bilayer structures which are separately optimized through DFT. Effects of atomic relaxation on the combined structure is investigated by optimizing the entire supercell again with the fixed lattice constants until the force on each atom are smaller than the threshold 0.01 eV/Å. From the comparison of band structures with (red) and without (black) atomic relaxation, atomic relaxation is found to have almost negligible effects on the overall band structures and the estimated band gap.

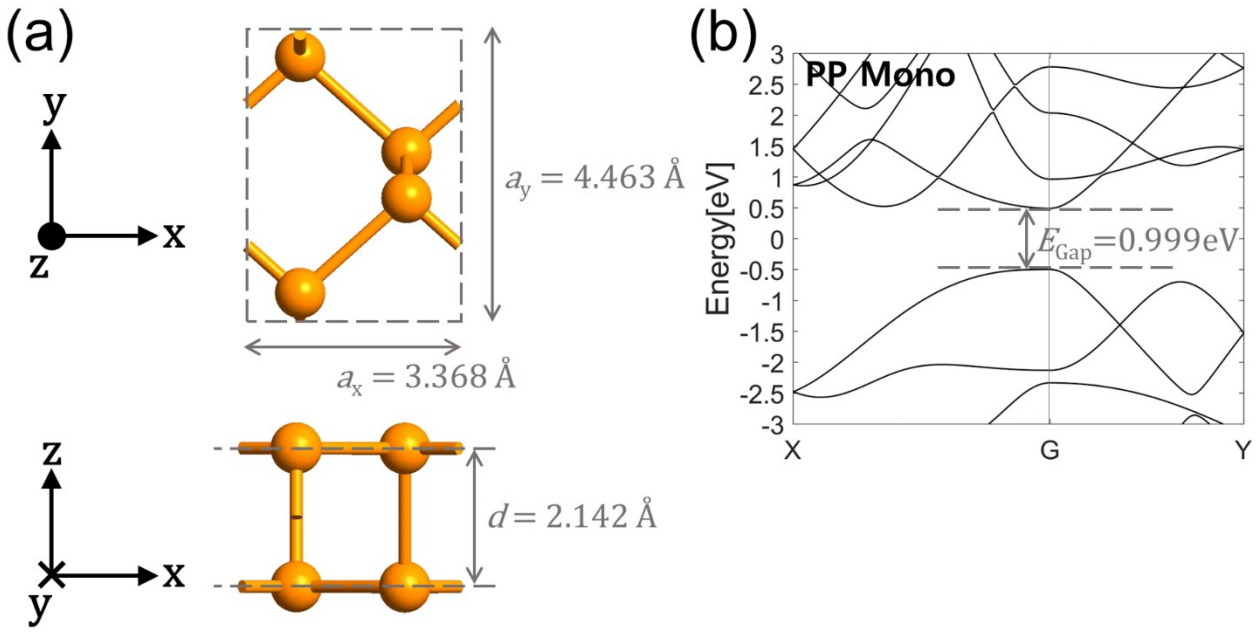

Figure S2. (a) Top and side views of phosphorene in primitive unit cell. (b) Band structure of monolayer phosphorene along the high symmetric paths in the 1st BZ.

Band structures of monolayer phosphorene are obtained from DFT calculations using GGA PBE functionals, FHI pseudopotential and DZP basis set. Troullier-Martins type norm-conserving pseudopotential set (FHI [z=5] DZP) is adopted for phosphorus. Geometry optimization of primitive unit cell is first performed with the force convergence criteria less than 0.01 eV/Å, leading to the equilibrium lattice constants of 3.368 and 4.463 Å for a_x and a_y, respectively, and the vertical interatomic distance d = 2.142 Å as in Figure S2(a). Calculate band structures are in Figure S2(b), well describing unique features of monolayer phosphorene: a direct band gap at Γ and anisotropic carrier effective masses near conduction band minimum and valence band maximum. Effective masses of both electrons and holes along the zigzag direction is about ten times larger than those along the armchair direction.