Supporting Information for

Enhancing electronic and optical properties of monolayer $MoSe_2$ via $MoSe_2$/Blue phosphorene heterobilayer

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Table S1 Calculated structural parameters and bandgaps of the monolayers and heterobilayers: lattice constants (a/b), bond lengths (l), interlayer distances (d), formation energies (E_f), and bandgaps at DFT-PBE ($E_{g\text{-}PBE}$) and G_0W_0 ($E_{g\text{-}G_0W_0}$) levels. "dir" and "ind" represent the direct and indirect of bandgap, respectively.

Name	a/b (Å)	$l_{P\text{-}P}$ (Å)	$l_{Mo\text{-}Se}$ (Å)	d (Å)	E_f (meV/unit)	$E_{g\text{-}PBE}$ (eV)	$E_{g\text{-}G_0W_0}$ (eV)
$MoSe_2$	3.322	——	2.549	——	——	1.44^{dir}	2.30^{dir}
Blue-P	3.269	2.271	——	——	——	1.92^{ind}	3.35^{ind}
AA-stacking	3.291	2.270	2.535	3.697	–211.9	1.15^{ind}	1.63^{ind}
AB_{Mo}-stacking	3.294	2.270	2.537	3.852	–185.4	1.12^{ind}	1.59^{ind}
AB_{Se}-stacking	3.288	2.269	2.535	3.809	–190.7	1.12^{ind}	1.58^{ind}

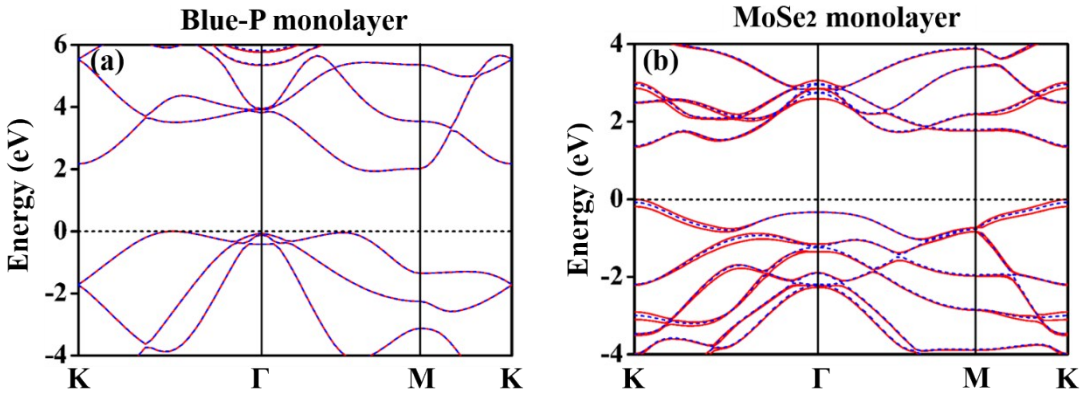

Fig. S1 Calculated band structures of monolayers with (red solid line) and without (blue dashed line) the spin-orbit coupling included at the DFT-PBE level: (a) Blue-P, (b) $MoSe_2$. The VBM is shifted to zero.

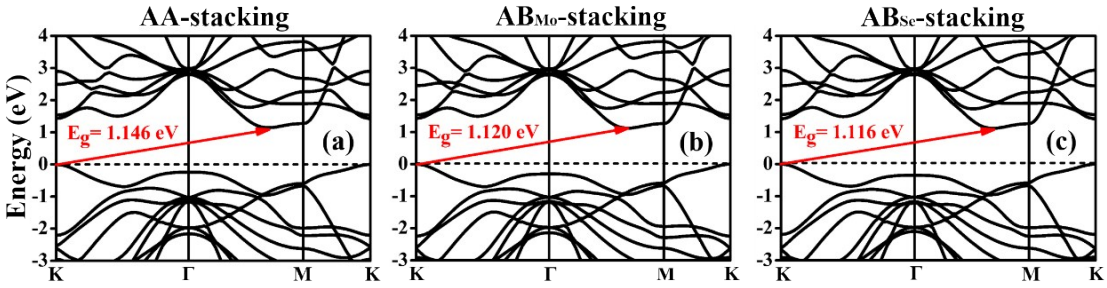

Fig. S2 Calculated band structures of $MoSe_2$/Blue-P heterobilayer at the DFT-PBE level: (a) AA-stacking, (b) AB_{Mo}-stacking, and (c) AB_{Se}-stacking. The VBM is shifted to zero.

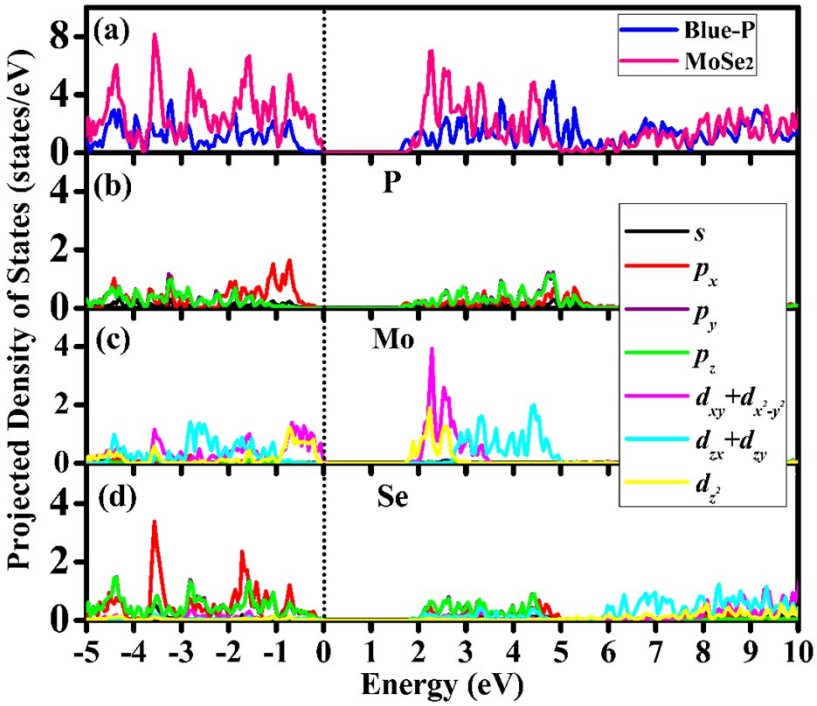

Fig. S3 (a), (b), (c) Projected density of states of the $MoSe_2$/Blue-P heterobilayer.

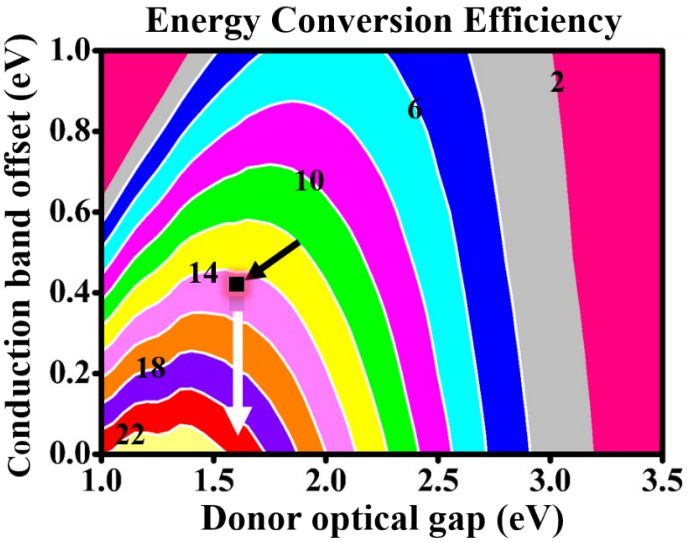

Fig. S4 Calculated energy-conversion efficiency contour as a function of the donor optical gap ($MoSe_2$ layer) and conduction band offset in $MoSe_2$/Blue-P heterobilayer. The white arrow indicates the trend of increase of energy-conversion efficiency through reducing the conduction band offset.