Donor Defect States of Monolayer and Bilayer Black Phosphorus

In Fig. S1 we show the five most strongly bound defect states for a positively charged adsorbate placed $d = 2$ Å above the top sublayer of monolayer black phosphorus on a substrate with (a) $\varepsilon_{\text{sub}} = 2$ and (b) $\varepsilon_{\text{sub}} = 8$. In Fig. S2 we show the wavefunctions of the donor adsorbate on freestanding bilayer BP.
Figure S1: Wavefunctions of the five most strongly bound donor states in monolayer black phosphorus on a dielectric substrate with (a) $\varepsilon_{\text{sub}} = 2$ and (b) $\varepsilon_{\text{sub}} = 8$, for a defect of height $d = 2 \text{ Å}$ above the top sublayer. All defect binding energies $E_{\text{bind}}$ are given relative to the conduction band edge.
Figure S2: Wavefunctions of the six most strongly bound states of donor adsorbates in bilayer BP in the top monolayer. Results for a positively charged adsorbate with $d = 2 \, \text{Å}$ above the top sublayer and $\epsilon_{\text{sub}} = 1$. Binding energies are given in the top left of each panel, relative to the conduction band edge. The wavefunctions in the bottom monolayer are shown in the inset.