

Supplementary Material: Electronic Structure of Monolayer and Bilayer Black Phosphorus with Charged Defects

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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 $d = 2 \text{ \AA}$ above the top sublayer of monolayer black phosphorus on a substrate with (a) $\epsilon_{\text{sub}} = 2$ and (b) $\epsilon_{\text{sub}} = 8$. In Fig. S2 we show the wavefunctions of the donor adsorbate on freestanding bilayer BP.

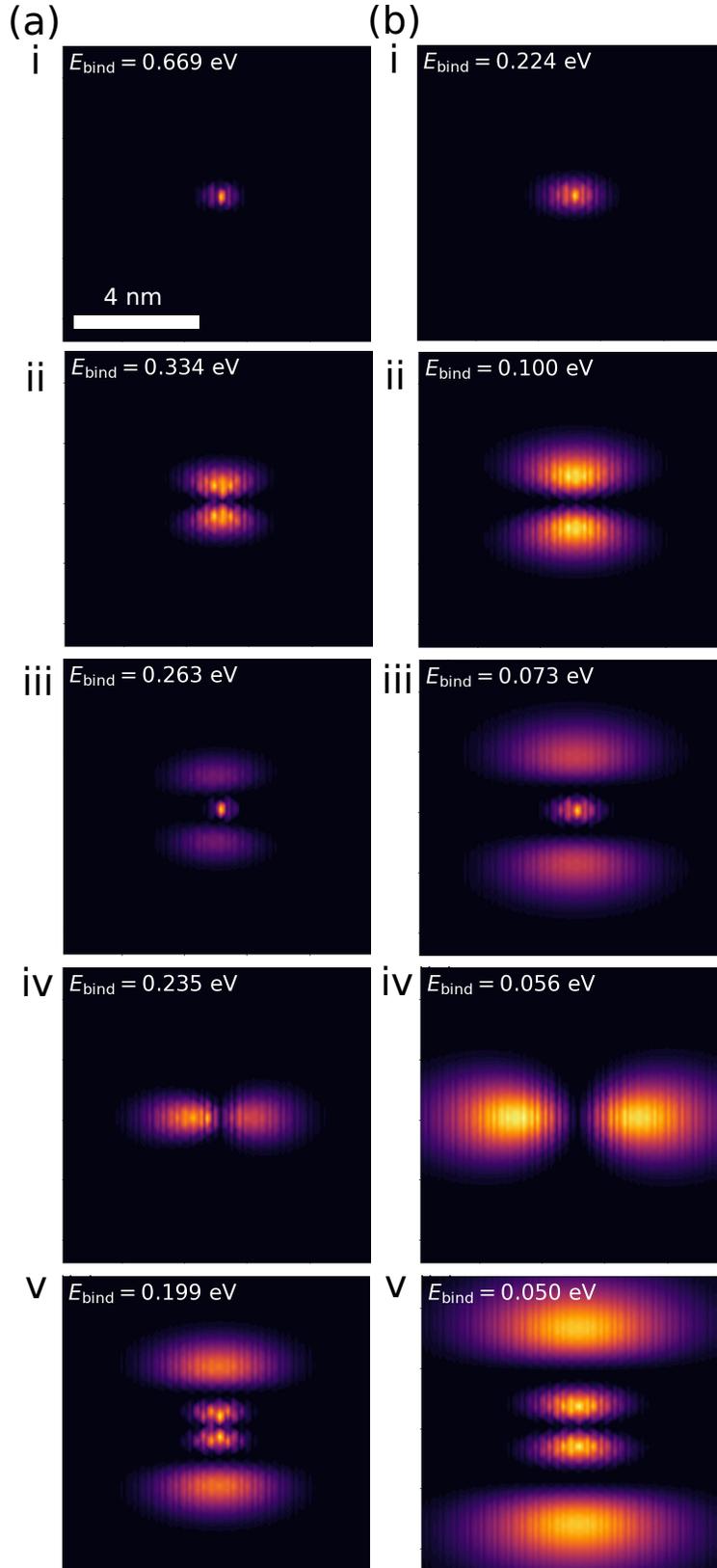


Figure S1: Wavefunctions of the five most strongly bound donor states in monolayer black phosphorus on a dielectric substrate with (a) $\epsilon_{\text{sub}} = 2$ and (b) $\epsilon_{\text{sub}} = 8$, for a defect of height $d = 2 \text{ \AA}$ above the top sublayer. All defect binding energies E_{bind} are given relative to the conduction band edge.

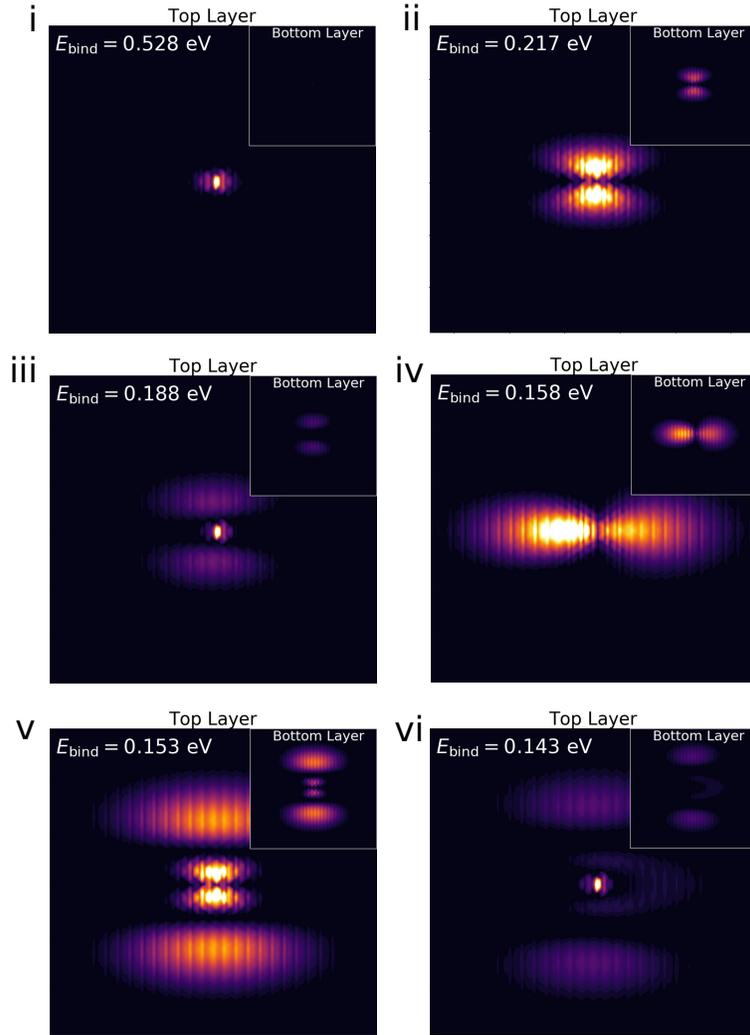


Figure S2: Wavefunctions of the six most strongly bound states of donor adsorbates in bilayer BP in the top monolayer. Results for a positively charged adsorbate with $d = 2 \text{ \AA}$ above the top sublayer and $\epsilon_{\text{sub}} = 1$. Binding energies are given in the top left of each panel, relative to the conduction band edge. The wavefunctions in the bottom monolayer are shown in the inset.