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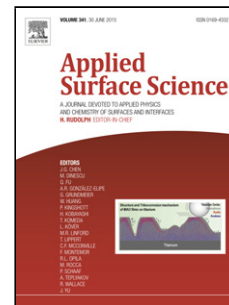
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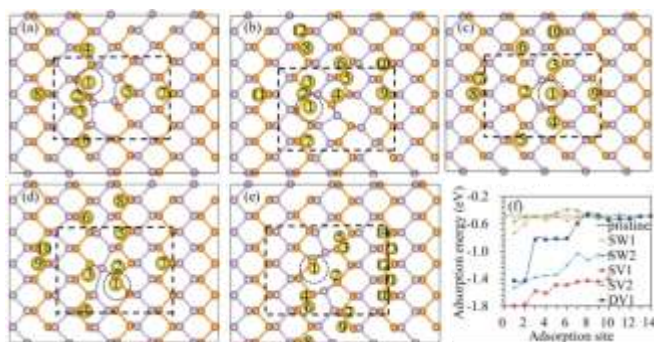
Sodium Adsorption and Diffusion on Monolayer Black Phosphorus with Intrinsic Defects

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GRAPHICAL ABSTRACT



HIGHLIGHTS

- Adsorption and diffusion of Na on phosphorus with defects were investigated.
- Defects enhance the adsorption of Na on monolayer black phosphorus.
- Defective phosphorus can be used as effective anode for SIBs.

ABSTRACT

Monolayer black phosphorus is a potential anode material for rechargeable ion batteries. In this work, the effects of intrinsic defects including mono-vacancy (MV), di-vacancy, and Stone-Wales (SW) defects on the adsorption and diffusion of sodium on monolayer black phosphorus were investigated using first-principles calculations. The adsorption energies for

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