Abstract Submitted
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First-principle study of the energy barrier and diffusivity of a Li atom on phosphorene CONGYAN ZHANG, MING YU, Univ of Louisville — The energy landscape of a Li atom adsorbed on the phosphorene was studied using the first principle method. Four types of preferential adsorption positions were found: three of them are located along the zigzag direction with the adsorption energy of -2.0˜-1.9 eV/atom, forming potential valleys along zigzag direction. The other type is located on the top of the puckered bridge with the adsorption energy of -1.4 eV/atom, forming small isolated shallow basins between the potential valleys. Based on this energy landscape, we calculated energy barriers along various diffusion paths. The lowest energy barrier is along the zigzag direction in the valley (0.09 eV). The highest energy barrier is along the armchair direction through the top of P atoms (1.01 eV). While the energy barrier on the top of the bridge along the zigzag direction and along the armchair direction through the P-P bonds are 0.20 eV and 0.79 eV, respectively. Estimated diffusivity along the zigzag direction in the valley is almost 10^{16} fast than that along the armchair direction through the top of P atoms, indicating the anisotropic diffusion.

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