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Anisotropic diffusion of oxygen on a few layers of black phosphorous. HECTOR NOE FERNNDEZ-ESCAMILLA, VCTOR HUGO GONZLEZ-CHVEZ, UNIVERSIDAD AUTNOMA DE NUEVO LEN, EDUARDO MARTNEZ-GUERRA, ANDRS GARAY-TAPIA, Centro de Investigacin en Materiales Avanzados, EDGAR MARTNEZ-GUERRA, UNIVERSIDAD AUTNOMA DE NUEVO LEN — Recently, phosporene has also been scored well as a functional material for two-dimensional electronic and optoelectronic devices. That is, because in contrast to graphene, black phosphorous has an inherent, direct and appreciable band gap that can be modulated with the numbers of layes. However, the presence of exposed lone pairs at the surface makes phosphorous very reactive to air and humidity and consequently, degradation of its properties. No such fundamental explanation have been made, thus corresponding first principle predictions to evaluate diffusion of O over and along a mono- and a few layers are indispensable. Energy barriers and the mechanisms of oxygen diffusion on mono- and a few layer of black phosphorous were calculated using the NEB(Nudge Elastic band) method as implemented in Quantum Espresso. The electronic states are expanded in plane waves with kinetic-energy cutoffs of 25 and 200 Ry for the wave function and charge density, respectively. Also, as the H_2O and O_2 are polar molecules, spin-polarized calculations have been carried out. We evaluated the diffusion barriers for O_2 and H_2O on phosphorene along zigzag, armchair and intermediated directions. Our calculations show that diffusion of O is preferred on zigzag directions and dissociation of O_2 is favored as a result of energy gains of about 2 eV. Also, apparently diffusion pathways are blocked along layers.

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