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Oxidation pathways in Phosphorene: an *ab-initio* investigation

MATHEUS PAES PAES LIMA, ADALBERTO FAZZIO, ANTONIO JOSE ROQUE DA SILVA, University of São Paulo — Phosphorene is a recently isolated single layer of Black Phosphorus. In this 2D material, the combination of a direct band gap with a high charge carrier mobility opens up the possibility of its use in nano devices. However, the exposure of Black Phosphorus to air leads to its fast degradation, which indicates the relevance to understand its oxidation processes. In the present work we investigate the initial steps of the oxidation process, focusing on the interaction of a single O_2 molecule with the phosphorene layer. We show the existence of oxidation pathways having only a single barrier of 0.13eV occurring between the free O_2 (triplet) and the triplet-singlet potential energy surface (PES) crossing point. We estimate a room temperature triplet-singlet transition probability of $P_{t \rightarrow s} = 0.015$, using the Landau-Zener model. Once the O_2 switches to the singlet PES, there is an oxygen incorporation with an energy gain of 4.2eV with respect to the PES crossing point, with the O_2 molecule spontaneously dissociating without any barrier. In this process, the final geometry has one O bonded to a P lone pair, and the other located between two P atoms. Our investigations were performed with DFT calculations at the GGA level as implemented in the VASP code.

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