Intrinsic Defects and Oxidation in Phosphorene: A Systematic Comparison to the Graphene

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Phosphorene, an exfoliated monolayer from black phosphorus bulk, has been extensively studied due to its remarkable electronic and mechanical properties, besides its high potential to application in optical-electronic devices. It has a direct gap at Γ point around 1.0 eV [1]. However, this material reacts strongly in the presence of oxygen and light [2], degrading after a short period of time. Unlike, graphene, an exfoliated monolayer from graphite, does not react to environmental contaminants so easily. Moreover, graphene is a null gap semi-metal and has high charge carrier mobility [3]. After the synthesis of these materials, they present intrinsic defects of atomic character [4,5], which can influence in the oxidation process.

In this work, we have performed a sistematic study on the stability of these materials, in pristine form or with intrinsical defects, subject to oxidation, in order to understand how this process occurs and whether the defects are an important factor in the oxidation. To do that, we have made use of the density functional theory (DFT), using electronic exchange-correlation PBE-GGA functional. We have made calculations for the pristine materials, phosphorene with 140 phosphorus atoms and graphene with 128 carbon atoms, subject to oxidation, as well as calculations with these materials subjects to Stone-Wales, simple (SV) and double (DV) vacancy defects, with and without oxygen incorporation. In order to understand how these materials oxidize and how this incorporation happens, we did several calculations of possible configurations in what this might take place. So, it was possible to have knowledge of which configurations are most stable. By formation energy calculations of defects and of the oxygen incorporation on the materials, we conclude that oxidation of phosphorene occurs in sites away from intrinsic defects because their presense do not diminish significantly the formation energy. In the case os graphene, there will be considerable oxidation only if the material presents high density of intrisic defects, since the formation energy to create a SV or DV defect is much larger than in the phosphorene case.

References: