

Abstract Submitted
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Graphene coatings: An efficient protection from oxidation MEHMET TOPSAKAL, HASAN SAHIN, SALIM CIRACI, UNAM-Institute of Materials Science and Nanotechnology — We demonstrate that graphene coating can provide an efficient protection from oxidation by posing a high energy barrier to the path of oxygen atom, which could have penetrated from the top of graphene to the reactive surface underneath. Graphene bilayer, which blocks the diffusion of oxygen with a relatively higher energy barrier provides even better protection from oxidation. While an oxygen molecule is weakly bound to bare graphene surface and hence becomes rather inactive, it can easily dissociate into two oxygen atoms adsorbed to low coordinated carbon atoms at the edges of a vacancy. For these oxygen atoms the oxidation barrier is reduced and hence the protection from oxidation provided by graphene coatings is weakened. Our predictions obtained from the state of the art first-principles calculations of electronic structure, phonon density of states and reaction path will unravel how a graphene can be used as a corrosion resistant coating and guide further studies aiming at developing more efficient nanocoating materials.

Mehmet Topsakal
UNAM-Institute of Materials Science and Nanotechnology

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