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Multi-Purpose Functionalization of Boron-Doped Graphene: insights from in silico experiments

We use DFT calculations to explore different kinds of functionalization of boron doped graphene and their possible applications describing their structures at atomistic level as well as providing information about their electronic properties. Exploiting our understanding of the "socket-plug" mechanism [1], we show that thanks to the doping with boron atoms it is possible to create dative bonds between the graphene surface and molecules with a lone-pair or metal surfaces. In particular, we envisage a possible use of graphene as a platform for custom-made receptors to create selective bio-sensors, for example for glucose in blood [2], as well as we describe its behavior as catalyst in NOx reduction [3]. Moreover, we show that the boron atoms can act as anchoring sites for a more efficient coating of metal surfaces enhancing the binding between the two materials and the resistance of the metal to corrosion, as it has been detailed for a copper surface [4-5]. Finally, we demonstrate how boron doped graphene can be used together with another 2D material, such as iron selenide, to create a novel heterostructure with enhanced superconductivity properties [6].

References

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