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Tuning the electronic, magnetic and optical properties of 2D materials: Ab initio insights

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The past decade has witnessed unprecedented advances in ab initio modelling of material properties. These advances have largely been attributed in part to algorithm refinements within codes implementing standard ab initio approaches such as density functional theory (DFT) and also to the advances made in high performance computing. It is thus now possible to model systems that were traditionally computationally expensive such as defects, extended surfaces and even nanoparticles. In this study the application of DFT to investigate the electronic, magnetic and optical properties of pristine and doped transition metal dichalcogenides (TMDCs), holey doped nitrogenated graphene g-C2N and graphene like GaN (g-GaN) is presented. Transition metal (TM) and lanthanide ion doping on the electronic, magnetic, optical properties of materials have also been taken into account. A more recent study on van der Waals hetero-structures/nanocomposites of graphene and graphene like AlN (g-AlN) for Li-ion battery (LIB) anode applications will also be presented in summary.

HPC content

Application of HPC in modeling materials' properties

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