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The Electric Field Gradient: A systematic Density Functional Study for Hg adatoms on Graphene

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Graphene is a two-dimensional (2D) atomic crystal which consists of a single graphite layer with strong covalent bonds between carbon arranged in a hexagonal lattice. Since it was isolated by André Geim and Konstantin Novoselov in 2004, graphene has become a remarkable subject of research, exhibiting novel phenomena that extend to virtually every domain of material's science and applications [1,2]. Engineering of graphene with specific chemical and physical properties predicts a revolution in electronics technology such as field-effect transistors, transparent electrodes, energy-storage materials, composites, chemical and biosensing, among others. Thus, modifying graphene in a controllable way is envisaged in this context and, particularly, adsorption of atoms (adatoms) on graphene could be used to tailor physical and chemical properties [3,4].

In this context, we present density functional theory (DFT) calculations analysing the interaction between graphene and Hg adatoms: hence atomic positions and stability, binding energies, electronic structure, and electric field gradients (EFG) are predicted in this way. Particularly, the EFG is highly sensitive to the signature of the atomic position with respect to the graphene layer, charge state, and type of bonding (ionic, covalent, van der Waals). These calculations, actually, form the interpretation basis for the experiments, which are currently being prepared at the ISOLDE facility at CERN, using the ASPIC (Apparatus for Surface Physics and Interfaces at CERN) [5] setup, and further prepare the interpretation and modelling of already performed experiments studying water molecules interacting with graphene and heavy metal ions.

References

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