The Magic of Interfaces: Organic Molecules and 4f Rare Earth Atoms Interacting with Graphene Substrates

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The density functional theory (DFT) proves to be the most practical theoretical framework that describes hybrid materials in a realistic manner. In this contribution I will show how *ab initio* studies based on DFT can be successfully employed to fundamentally elucidate and explain a large variety of surface-science measurements. Furthermore, I will demonstrate that due to its predictive power, the DFT (i) represents a fundamental theoretical engine that essentially guides the experiments and (ii) is a pathfinder in designing novel materials.

For example, when graphene adsorbs on metal substrates the subtle interplay between the electrostatic, the weak van der Waals and the strong chemical interactions can be precisely manipulated by intercalation and crystallographic surface termination. In turn, this leads to graphene patches with different reactivities that can be easily used to select the reaction path in on-surface chemical synthesis and uniaxially align 1D sandwich molecular wires.

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