Ab initio Simulations of Organic Molecules and 2D Systems Interacting with Magnetic Surfaces

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The density functional theory provides a framework with predictive power that can be used to describe hybrid systems in a realistic manner. In this respect, *ab initio* studies elucidate how the subtle interplay between the electrostatic, the weak van der Waals and the strong chemical interactions determine the geometric, electronic and magnetic structure of hybrid interfaces formed between organic molecules and 2D materials with metallic surfaces. More precisely, the interaction between the π-like electronic cloud of organic materials or the lone electron pairs of the 2D systems with the magnetic states of a metal influences the (i) spin-polarization, (ii) magnetic exchange coupling, (iii) magnetic moments and (iv) their orientation at the hybrid interfaces. In this contribution I will briefly summarize how first-principles calculations (i) provide the basic insights needed to interpret surface-science experiments and (ii) are a key tool to design novel materials with tailored properties that can be integrated in spintronic devices.

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