WWU MÜNSTER

FACHBEREICH PHYSIK

Allgemeines Physikalisches Kolloquium

Donnerstag, 08.12.2022 um 16 Uhr c.t.

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The Magic of Interfaces: Organic Molecules and 2D System Adsorbed on Metals and Magnetic Substrates

Theoretical simulations based on the density functional theory provide a framework with predictive power that can be used to describe hybrid materials 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 and magnetic substrates. 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. I will briefly summarize how first-principles calculations (i) provide the basic insights needed to interpret surface-science experiments and most importantly (ii) represent a key tool to design novel materials.

References:
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