Sonderforschungsbereich 1277

Emergent Relativistic Effects in Condensed Matter -
From Fundamental Aspects to Electronic Functionality

SFB – Seminar

Speaker: **Dr. Rémi Pasquier**

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Date: Friday, 05.04.2024, 10:30, PHY 5.1.34 B

Topic: Theory of Spin Crossover Molecules on Metal Surfaces

Abstract:

This work consisted in the use of Ab-initio DFT methods within the VASP package to study the physics of spin-crossover molecules adsorbed on metallic surfaces, systems of high experimental interest because of their wide range of potential applications in spintronics (e.g. to create qubits in quantum computing). Several aspects of the subject were theoretically investigated, including the effects of doping on the spin-crossover phenomenon, calculation of the x-ray absorption spectra through a personal implementation within VASP or scanning tunnel microscopy images beyond the Tersoff-Hamann approximation.

Host: Dr. Jan Wilhelm