Postdoctoral research position at CEA-Saclay, France

DFT modelling of spin-crossover complexes for molecular spintronics applications.

A 18-month postdoctoral position is open in the laboratory of Physics of the Condensed State (SPEC: Service de Physique de l’état condensé) at CEA-Saclay.

**Subject description:**
In molecular spintronics besides the rich magnetic behavior resulting from the interaction between a magnetic molecule and a metal surface, or vice versa, additional functions such as switchability by external parameters (light, voltage) can be integrated. Spin cross-over (SCO) molecules are promising systems as they present two (low and high) electronic spin states that can be controlled by external stimuli such as light, pressure, temperature or electric field.

In this position we focus on the theoretical (DFT based) modelling of SCO complexes deposited on a metallic surface. We will in particular study the influence of intermolecular interactions as well as molecule-substrate interaction on the relative stability of the low and high-spin state. The final goal is to incorporate these molecules in a molecular junction through which an electric current will pass. This work will involve a close collaboration with theory/modelling groups in Denmark, DTUnano and Synopsys-Denmark Software Company and experimental groups in Paris, Kiel and Valencia.

This is a position within a European network of 6 partners, aiming at the development and use of modelling tools for molecular spintronics guided by well-controlled and calibrated experiments. In particular, we aim at devices where the spin transport can be controlled by an external stimulus (e.g. light or electronic current/field).

**Skill requirements:**

Applicants should hold a PhD degree in Solid State Physics, Materials Science or Quantum Chemistry or a closely related discipline, with a strong background in condensed matter and Density Functional Theory (DFT), preferably with experience in nano-scale magnetism. Experience in transport calculations based on non-equilibrium Greens functions (NEGF) is a plus. We also prioritize candidates with a track-record proving successful collaborations with experimentalists since this is central to the project.

Applicants should provide a CV, a list of publications and at least two reference letters.

**Contacts:**

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