



Laboratoire de Chimie et Physique
Quantiques
Université Paul Sabatier - CNRS UMR 5626



Post-doctoral fellowship

Methodology and Applications for Magnetic Anisotropy in Polynuclear Complexes

Job description

In the framework of the French ANR research project SMolMagIC (Switchable Molecular Magnets for Quantum Information), a post-doctoral position is proposed in theoretical chemistry at LCPQ, Toulouse, France, for highly motivated candidate interested in methodology and applications in magnetism.

Context of the project

This post-doc is funded by the French ANR SMolMagIC project. The candidate will be joining the Extended Systems and Magnetism team of LCPQ. This research will be conducted in the context of an ongoing collaborations between LCPQ, ICMMO (Paris-Saclay) and LNCMI (Grenoble).

Scientific project and objectives

During the past decade, we have developed and tested a now well-established technique to determine magnetic anisotropy parameters on mononuclear systems. Recent studies enabled us to study polynuclear compounds and it appears that new methodologies are required to describe precisely the polycentric interactions. Methodological developments and implementation of a new code will be the main part of the project. In the context of the collaborations with synthetic chemists and specialists in EPR spectroscopy, this methodology will be applied to a series of new systems with potential applications of interest in the domain of quantum computing.

Requirements

PhD in theoretical chemistry, experience with wave function based methods, strong programming skills, solid analytical ability, and high motivation.

Submit your CV and motivation letter at: nathalie.guihery@irsamc.ups-tlse.fr and nicolas.suaud@irsamc.ups-tlse.fr

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