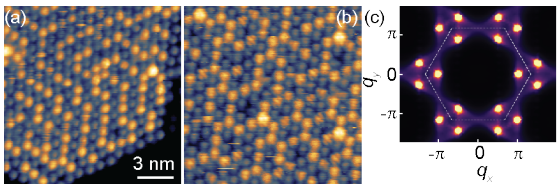
NÉEL INSTITUTE Grenoble

Topic for Master 2 internship – Academic year 2022-2023

Emulating frustrated spin Hamiltonians with molecular lattices

General Scope: In 1935, Linus Pauling explained why ice crystals exhibit residual entropy, even down to absolute zero. This property contradicts the third law of thermodynamics (at least in its often-taught formulation) and stems from the positional (local) disorder of the protons within the oxygen crystal [1]. Since then, physicists have found formidable playgrounds in ice-like systems, with which exotic states of matter and unconventional phenomena can be be studied. For instance, in magnetic and artificial analogues of ice, we unveiled, directly in real space, the existence of massively degenerate and disordered ground states violating the third law [2]. Very recently, in the framework of a Ph.D. thesis now ending, we have reconsidered Pauling's viewpoint and demonstrated that two-dimensional layers of fullerene (C_{60}) molecules (see figure) also exhibit striking analogies with water ice [3] and proved to be a fascinating platform to challenge the third law. Besides, seminal predictions from frustrated spin Hamiltonians can actually be directly tested and revisited using such molecular layers. The panel of exotic phases and unconventional collective behaviours that can be investigated accordingly appears considerable.



(a,b) Frustrated lattices of C_{60} molecules imaged by scanning tunneling microscopy. (c) Magnetic structure factor, calculated for a model Hamiltonien describing (b).

[1] L. Pauling, *Journal of the American Chemical Society*, vol.57, p.2680 (1935).

[2] Y. Perrin, B. Canals, N. Rougemaille, *Nature*, vol.540, p.410 (2016). — B. Canals *et al*. *Nature Communications* 7, 11446 (2016)

[3] M. Alfonso-Moro *et al*., Corrugation in a molecular C_{60} monolayer as a spin liquid candidate. — M. Alfonso-Moro *et al*., Coexisting metal-fullerene surface alloys: local three-dimensional strains and rotations, order/disorder. *Articles soon published*

Research topic and facilities available: The project focuses on frustrated spin Hamiltonians in which exotic phases of matter and non-conventional phase transitions are expected, possibly in connection with topological properties. We will also investigate potential experimental means to manipulate the molecular assemblies at the level of individual molecules, seeking to trigger global changes and understand to what extent local excitations propagate. Our approaches are both experimental (scanning tunneling microscopy, cf. figure) and theoretical, relying on Monte Carlo simulations and analyses of the thermodynamic properties of the systems of interest.

Possible collaboration and networking: The work will rely on strong interactions with several researchers from Institut Néel, who are experts in the physics of frustrated spin systems and in the study of molecular layers on surfaces. The student will hence be involved in strongly collaborative working and will benefit from significant technical support. Besides, high resolution microscopy measurements are envisaged, in the framework of a collaboration with another laboratory.

The internship can lead to a PhD project

Required skills: Strong background in solid state physics and statistical physics.

Starting date: Spring, 2023

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More information : http://neel.cnrs.fr