PHD PROJECT DESCRIPTION

(4000 characters max., including the aims and work plan to de published online)

Project title:

1.1. Project goals

The project goals aim at designing spin models from open-shell nanographenes in order to create realistic quantum simulators [1]. Open-shell nanographenes characterize by nonzero magnetic moments, or no net magnetic moment but antiferromagnetic coupling [2]. Using advanced quantum mechanical tools, we will determine conditions for realization of spin models from nanographenes that include one dimensional chains with half-integer and integer spins, finite size spin systems and two-dimensional crystals.

1.2. Outline

Exact analytical solutions have been developed for relatively simply microscopic quantum models supported by powerful field theoretic and computational approaches, providing greater insight into the emergence of these complex phases and their physical properties. Understanding of spectral and topological properties of various quantum mechanical correlated models is challenging due exponential growth of Hilbert space with a system size, while experimental investigation of such systems might answer to crucial questions regarding fundamental laws governing the quantum world. This approach belongs to a general class of quantum simulations [1]: designing quantum mechanical systems that mimic the other ones that cannot be solved neither numerically using standard (classical) computers, nor using analytical methods. On-surface synthesize has led to the discovery of open-shell nanographene as promising building blocks for creating quantum spin models [2]. Recent fabrication of synthetic spin 1 chain with characteristic edge states of Haldane symmetry-protected topological phase [3] open a bottom-up approach to study strongly correlated topological phases in purely organic materials. Synthesized carbon nanostructures of various shapes allow one to create systems with magnetic order and controllable magnetic exchange coupling. Realization of isotropic spin ½ chain designed in nanographenes and observation of spinons show huge potential in these quantum simulators [4-6]. We plan to utilize several atomistic many-body approaches to investigate electronic properties of nanographenes and to map their low spectrum to effective spin models.

1.3. Work plan

We will start from already implemented tight-binding, Hartree-Fock and exact diagonalization methods to derive accurate fermionic model of various nanographenes. This will allow us to investigate the basic properties of the systems. Next, we will determine parameters of effective spin models by direct comparison of low energy spectra. We will realize different spin models from nanographenes that include one dimensional chains with half-integer and integer spins, finite size spin systems and two-dimensional crystals. Next, we will relate our findings to the experiments. Demonstration the Haldane gap and topological edge states [3] of one-

dimensional spin-1 chains made of pi-electron magnetic nanographene highlighted the potential of combined on-surface synthesis and STM atomic detection. Scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) are used to characterize and manipulate spin degrees of freedom. Spin excitations can be probed using inelastic electron tunneling spectroscopy (IETS). In the conventional theory for IETS, the zero bias conductance is related to the square of the local magnetization of the ground state through resonant tunneling via the Kondo effect. We will model the dI/dV spectroscopy following Ref. [7]. Electron scattering that can produce a spin flip can be related to electrons that tunnel from tip to sample, exciting from the ground state in the process, and scattering between the substrate electrons. We will confront our simulations of STM spectra with the latest experiments.

1.4. Literature (max. 7 listed as a suggestion for a PhD candidate preliminary study)

[1] R. Feynman, Int. J. Theor. Phys. 21, 467 (1982).
[2] D. G. de Oteyza and T. Frederiksen, J. Phys.: Cond. Mat. 34, 443001 (2022).
[3] S. Mishra et al. Nature 598, 287–292 (2021).
[4] Z. Yuan et al. J. Am. Chem. Soc. 147, 6, 5004–5013 (2025).
[5] X. Su Nature Synthesis 4, 694–701 (2025).
[6] C. Zhao et al. Nature 24, 722-727 (2025).
[7] J. Fernández-Rossier, Phys. Rev. Lett. 102, 256802 (2009).

1.5. Required initial knowledge and skills of the PhD candidate

- MSc in physics.
- Fundamental knowledge about quantum mechanics.
- Basic experience in many-body quantum mechanical calculations
- Basic experience in lattice models will be an advantage
- Skills in computer programming (C, Matlab, Python or Fortran)
- Communication skills and ability for working in a team
- English in speaking and writing (advanced)

1.6. Expected development of the PhD candidate's knowledge and skills

- practical skills and expert knowledge in the field of nanostructure theory and spin models
- practical understanding of quantum many-body effects
- experience in high-performance computation
- ability to write scientific papers in English
- ability to present results of own research in a professional manner
- teamwork skills