Postdoctoral Position in Theoretical Condensed Matter Physics or Theoretical Chemistry

L'Institut des NanoSciences de Paris
Sorbonne Université
Paris 75005

Applications are invited for a postdoctoral research position to explore the electronic structure and non-equilibrium photodynamics of novel low-dimensional organic materials. The work is particularly focussed on real-time dynamics and spatiotemporally resolved spectroscopy of excitons and spins, and their eventual exploitation in optoelectronic and quantum information applications.

The post is part of the 4-year ANR project (ACCEPT) and a new 5-year project between the INSP Theory Group and experimentalists at the University of Cambridge (Rao Group) [1, 2]. The initial phase of the work will be supervised by Dr Alex W Chin (Sorbonne université), Davide Romanin (Paris-Saclay) and Prof Matteo Calandra (Trento Université).

Applications are particularly encouraged from candidates who would be able to contribute to one or more of the follows aspects of the project :

1. First principle simulations of the electronic and vibrational structure of low-dimensional organic semiconductors synthesized by emerging 'on surface' techniques and topochemical methods [3, 4].

2. Using many body perturbation methods (GW, BSE..) to predict the optical and excitonic properties of these structures, and also the coupling of singlet and triplet excitons to phonons and (radical) spin centres [5].

3. Computation of the dissipative, real-time dynamics of excitons and spin excitations that could be observed with emerging ultrafast microscopy methods [6]. This work will be based around the many body tensor network methods that are under active development in the Chin Group [7, 8].

The work will be conducted in the Photonics and Coherence of Spin Group at the Paris Institute of Nanosciences (L'institut des Nanosciences de Paris), which is situated right in the heart of Paris' Latin quarter. Candidates should possess a strong background in quantum mechanics and condensed matter theory/theoretical chemistry, and also have research-level experience of density functional methods and/or numerical tensor network techniques. Applications would also be considered from candidates with a strong background in open quantum systems and related numerical techniques, such as non-Markovian master equations, or path integral methods.

The position is due to start by the end of June 2023 and is available for 24 months. Applicants should contact Dr Alex Chin at alex.chin@insp.upmc.fr, including a CV and a list of any relevant publications.

References

[1] `https://anr.fr/Project-ANR-19-CE24-0028`.

[2] `https://anr.fr/Project-ANR-22-CE30-0033`.

[3] D Romanin, M Calandra, and Alex W Chin. Excitonic switching across a z 2 topological phase transition: From mott-wannier to frenkel excitons in organic materials. *Physical Review B*, 106(15):155122, 2022.

[4] Davide Romanin and Matteo Calandra. Giant quantum anharmonic effects on the stability, vibrational and optical properties of cyclo [4n+ 2] carbon. *Carbon Trends*, 9:100207, 2022.

[5] Raj Pandya, Qifei Gu, Alexandre Cheminal, Richard YS Chen, Edward P Booker, Richard Soucek, Michel Schott, Laurent Legrand, Fabrice Mathevet, Neil C Greenham, et al. Optical projection and spatial separation of spin-entangled triplet pairs from the s1 (21 ag–) state of pi-conjugated systems. *Chem*, 6(10):2826–2851, 2020.

[6] Raj Pandya, Richard YS Chen, Qifei Gu, Jooyoung Sung, Christoph Schnedermann, Oluwafemi S Ojambati, Rohit Chikkaraddy, Jeffrey Gorman, Gianni Jacucci, Olimpia D Onelli, et al. Microcavity-like exciton-polaritons can be the primary photoexcitation in bare organic semiconductors. *Nature communications*, 12(1):6519, 2021.

[7] Angus J Dunnett, Duncan Gowland, Christine M Isborn, Alex W Chin, and Tim J Zuehlsdorff. Influence of non-adiabatic effects on linear absorption spectra in the condensed phase: Methylene blue. *The journal of chemical physics*, 155(14):144112, 2021.

[8] Angus J Dunnett and Alex W Chin. Efficient bond-adaptive approach for finite-temperature open quantum dynamics using the one-site time-dependent variational principle for matrix product states. *Physical Review B*, 104(21):214302, 2021.