SCIENCES SORBONNE UNIVERSITÉ

2021-2022

Master thesis proposal

INSP INSTITUT DES NANOSCIENCES DE PARIS

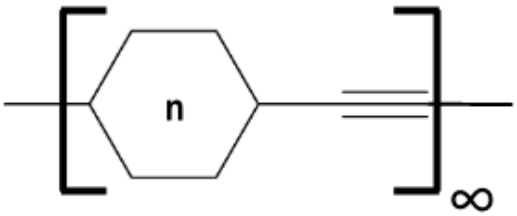
Campus Pierre et Marie Curie
Tower 23 – 3rd floor – 23-22
Director: Massimiliano Marangolo

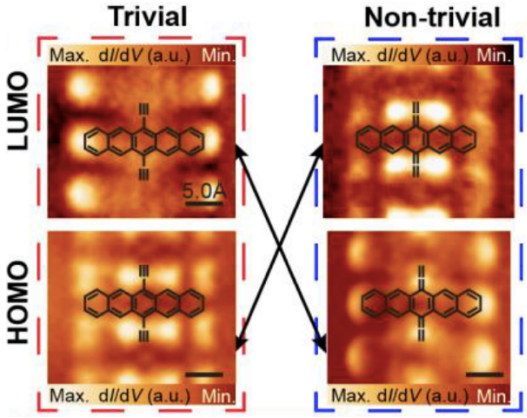
Title: *Optical properties of topological insulating polymers*

Keywords: one-dimensional systems, many-body interactions, topological insulators, Bethe-Salpeter, excitons, singlet fission, numerical simulations

Scientific description:

In recent papers (Refs. [1]-[2]) it was shown that it is possible to observe a topological phase transition in 1D acene ethynylene-bridged polymers from a trivial to a non-trivial insulating phase as a function of the monomer acene size (n). Combining tight-binding, DFT and GW calculations they showed that such quantum phase transition was accompanied by an ethylenic-to-cumulenic transition in the molecular bridges between the acenes, and that the presence of a topological transition could provide a route to novel organic metals.





However, the optical properties of such polymers and the impact of the topological transition on their excitonic excitations were not discussed. We therefore propose to study the excitonic properties of infinitely extended pi-conjugated acene ethynylene-bridged polymers both in the trivial and non-trivial quantum phase. Moreover we plan to study to which extent it is possible to approach the quantum critical point by tuning the relevant degrees of freedom and to study the effects on the optical response. This latter part opens the possibility of further exploration of how these non-trivial properties might be applied in next-generation optoelectronics devices, such as singlet-fission based solar cells.

[1] B. Cirera et al., "Tailoring topological order and pi-conjugation to engineer quasi-metallic polymers", Nature Nanotechnology 15, 437-443 (2020).
[2] H. Gonzàlez-Herrero et al., "Atomic scale control and visualization of topological quantum phase transition in π-conjugated polymers driven by their length", arXiv:2105.00025 [cond-mat.mes-hall] (2021).
[3] Korovina *et al.*, Nature Chemistry volume 12, 391–398 (2020)

Techniques/methods in use: Density Matrix Renormalization Group (DMRG), Density Functional Theory (DFT), Many-Body corrections.

Applicant skills: A strong background in solid state physics, as well as interest and experience of scientific computational languages (Fortran, C++, Python, Julia) would be highly advantageous.

Industrial partnership: No

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Possibility for a Doctoral thesis: Yes, subject to funding