Internship offer 2023/2024

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Theoretical Investigation of Topologically Insulating Polymers for Energy Applications

Scientific project: Generally speaking, π-conjugated organic semiconductors form a highly versatile class of materials with tremendous promise for the development of cheap, flexible and non-toxic optoelectronic devices such as photovoltaics, sensors and solid state lighting [1].

One of the ultimate frontiers in energy conversion and storage from light-matter interactions is to create long-lived excitonic quasiparticles (bound electron-hole states in semiconductors) [2]. Topological insulators represent an ideal platform for this, as they show correlations between spatial separation and topological surface states [3].

Experimental evidence for a topological (Z2) phase transition has recently been presented in a series of 1D polyacene polymers, representing a physical realisation of the well known Su-Schrieffer-Heeger (SSH) model [4].

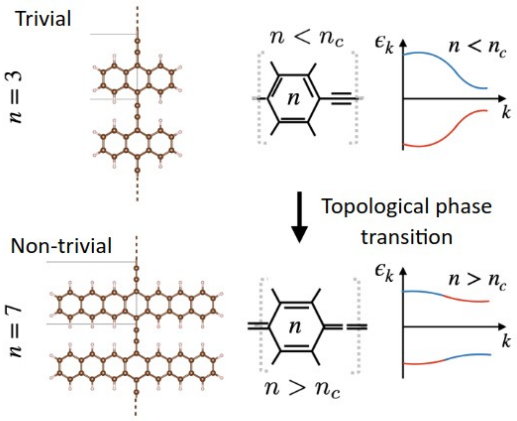
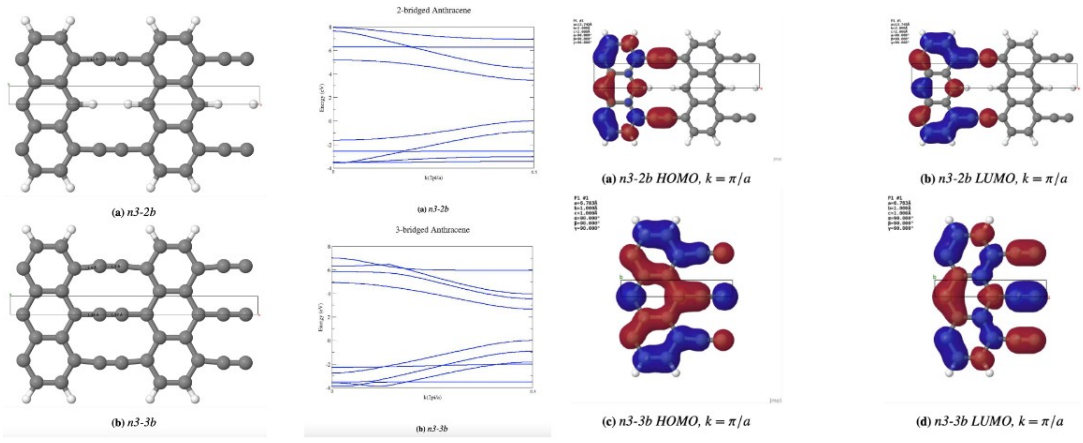


Fig. 3 : Topological phase transition of polyacene polymers [19]

The student will rationalise an analytical effective model by calculating the topological invariants of different bridged configurations through an-initio computational techniques. After that we will select the suitable candidates (at least 2, one trivial and one non trivial topological phase for the master student) for the computation of the optical properties, i.e. with quasi-particle band gaps and excitons via many-body theoretical techniques.



[1] H. Bronstein, et al., Nature Reviews Chemistry 4, 66 (2020)
[2] H. Luo, et al., Nat Rev Phys 4, 611–624 (2022)
[3] T. Cao et al., Phys. Rev. Le[. 120, 087402 (2018)
[4] D. Romanin, et al., Phys. Rev. B 106, 155122 (2022)

Methods and techniques: Density Functional Theory (DFT), Density Functional Perturbation Theory (DFTP), Wannier Functions, Bethe-Salpeter Equation

Student profile: We are looking for master students with a strong background in solid state physics as well as knowledge of electronic structure theory and computataional languages (Fortran, C++, Python, Julia). Previous experience of DFT codes (e.g. Quantum ESPRESSO) would be advantageous.

Possibility to go on with a PhD ? Yes, with funds from Agence Nationale de la Recherche (ANR)