M2 Stage proposal

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Title: Theoretical Electronic Structure and Excitonic Properties of *Organic* Topological Semiconductors

Keywords: Exotic topological band structures of 1D organic polymers and metals; strain tunable optical and transport properties; excitonic insulators; DFT and many body numerical techniques; cluster computing, quantum condensed matter theory

Scientific description:
Band topology is now considered to be as fundamental as band structure, underlying emergent quasiparticle phenomena such as robust edge states and spin-chain physics in organic systems (e.g. graphene nanoribbons), but the impact of topological band structures on the physics of excitons (i.e. a correlated electron-hole photo-excited state bound by Coulomb interaction) has only recently begun to attract widespread attention. Understanding and controlling the effects of topological phase transitions on the electronic and optical responses of materials could become a powerful tool for the design of novel optoelectronic devices and future quantum technologies, and this project will explore an exciting new class of organic 1D materials in this context.

Experimental evidence for a topological (Z2) phase transition has recently been presented in a series of 1D polyacene polymers (see Fig. 1) in which the monomer size and chain length could be systematically varied [1,2,3], representing a physical realization of the well-known Su- Schrieffer-Heeger (SSH) model [1,3]. This transition is associated with a dramatic closing and reopening of the polymer quasiparticle gap, as the size of the monomer increases. However, the 'tuning' parameters (monomer size and chain length) controlling the topological properties are discrete (step-like) in nature, making it hard to explore the emergent physics right at the critical point/phase transition itself. In this project, we will explore how a continuous tuning parameter – strain – can be used to drive these polymers to the point where the band gap closes and elucidate the nature of the critical state (metal? Excitonic insulator?...). This will be accomplished through training and employment of state-of-the-art computational methods for simulating the electronic, phononic and excitonic structure of strained systems at a truly atomistic, *ab initio* level of theory.

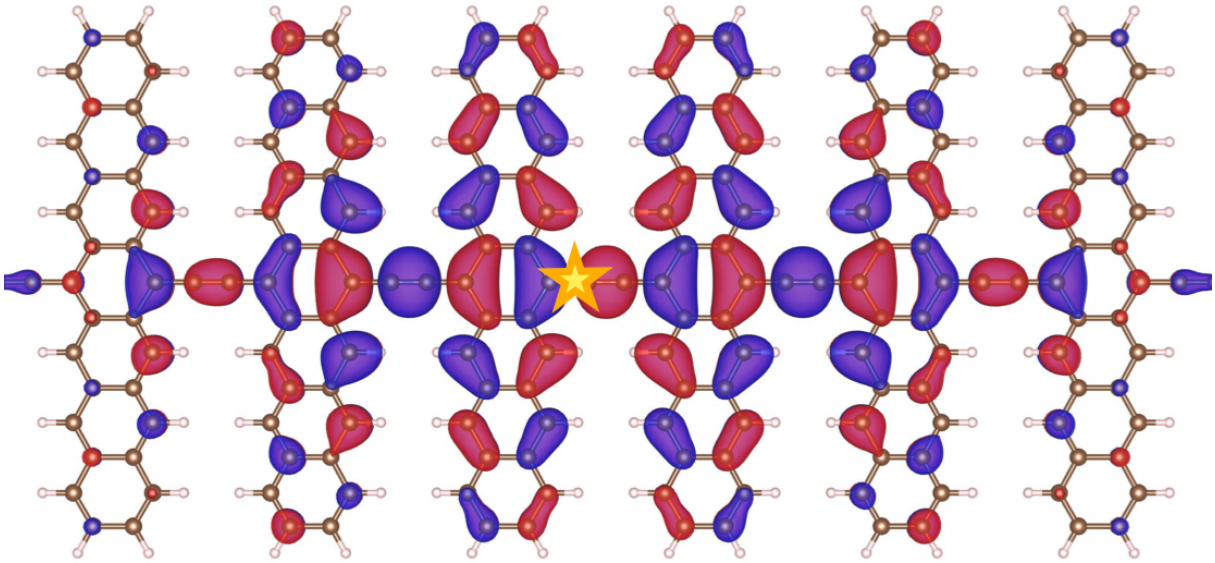

Figure 1. The electronic wavefunction associated with a fixed, point-like hole (star) in the lowest energy, optically allowed exciton of the topologically non-trivial material polyheptacene.

Refs: [1] Nature Nanotechnology 15, 437 (2020): [2] Adv. Mater. 33, 2104495 (2021): [3] Physical Review B 106 (15), 155122 (2022)

Techniques/methods in use: Numerical algorithms for electronic structure and geometry simulations (DFT); advanced many body perturbation theory codes to describe electron-electron interactions and strong electron-hole correlations (excitons); tight-binding methods and analytical/physical analysis of results.

Applicant skills: strong theoretical and computational background in quantum mechanics; experience of using open parallel computing codes using open MPI or similar would be especially welcomed, but is not a prerequisite; ability to effectively manage data; ability to work collaboratively in an independent and team setting; advanced level in English would be an advantage (due to ongoing collaborations with our international partners in Cambridge (UK), Princeton (US), Oregon (US), Saint Andrews (UK) and many other anglophone partners across Europe).

Industrial partnership: N

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