University of Cyprus
Department of Physics

The Department of Physics at the University of Cyprus announces

PhD Thesis Defense Seminar by
Georgia Polycarpou

Thursday April 10th 2025, 11:30am (Cyprus time)

Room B228 Department of Physics

"COMPUTATIONAL AND THEORETICAL STUDIES OF BIOMOLECULAR CHARGE TRANSFER"

This PhD dissertation investigates charge-transfer mechanisms in biomolecular systems using numerical simulations, ab initio computations, and MD simulations. The first part deals with interpreting charge transport measurements through dry 30-nm-long double-stranded DNA molecules[1,2]. The experiments observe currents of the order of tens of nanoamperes for dsDNA molecules that differ in their base-pair sequences. The introduction of a single discontinuity in each of the DNA backbone strands leads to a complete suppression of the current. This suggests that the backbone may mediate long-distance conduction in dsDNA in the particular experiments, contrary to the common wisdom in DNA electronics. I describe extensive molecular dynamics simulations coupled with electronic structure computations that support the idea of backbone conduction via an incoherent hopping mechanism. Then, I explore the circumstances under which the backbone may dominate long-distance DNA charge transport. I show that the degree of solvation can determine the participation of backbone orbitals in charge transport. Solvation affects the level of dynamic disorder in the pi-stacking between bases, and also the energies of phosphate-group molecular orbitals. The lower the solvation shell, the more important the backbone becomes for charge transport as compared to the bases. The second part of the thesis deals with cable bacteria that are filamentous, multicellular organisms that exhibit a unique form of biological electron transport over centimeter-scale distances. The currents are channeled through a network of Ni-bis(dithiolene)-type protein fibers within the cell envelope. The fibers have extraordinary electrical properties for a biological material, including an electrical conductivity of up to 100 S/cm. These features have triggered intriguing questions about the precise molecular structure and mechanism of centimeter-scale conduction of the cable-bacterium protein fibers. I describe computational and theoretical work that explores how Ni-bis(dithiolene) molecules would perform as electron-donor and acceptor centers in protein-mediated charge transfer.[3] This work gives upper bounds for donor-to-acceptor rates mediated by the protein, as a function of molecular redox state and structure, and as a function of protein bridge sequence. The work is relevant to both biological protein electron transfer chains and to the design of artificial protein wires that incorporate these Ni-bis(dithiolene) molecules as redox cofactors.

1. Zhuravel, R.; Huang, H.; Polycarpou, G. et al. *Nat. Nanotechnol.*, 15, 836-840, 2020
2. Polycarpou, G; Skourtis S. S. *J. Phys.: Condens. Matter*, 36, 375301, 2024
3. Polycarpou, G; Skourtis, S. S. *J. Phys. Chem. B*, 129, 2992-3006, 2025

The seminar is open to the public.

Για περισσότερες πληροφορίες παρακαλώ επικοινωνείτε: Τμήμα Φυσικής, τηλέφωνο: 22892820