Πανεπιστήμιο Κύπρου
Τμήμα Φυσικής

Το Τμήμα Φυσικής του Πανεπιστημίου Κύπρου
σας προσκαλεί την

Πέμπτη, 15 Δεκεμβρίου 2022, ώρα 11:00
στην αίθουσα Β228, στο κτίριο 13 στην Πανεπιστημιούπολη

στην παρουσίαση της Διδακτορικής Διατριβής της Σπυρούλλας Μαυρομμάτη

"Simulations of molecular transitions involving spin, charge and energy transformations"

This PhD thesis describes research work on triplet energy transfer (TET) and charge transfer (CT) processes in molecular systems. The first part relates to unusual experimental observations of time-resolved electron paramagnetic resonance (TR-EPR) spectra of an organic molecule. The EPR spectra following optical excitation within a highly absorbing region of the molecule have similar intensities as the EPR spectra following optical excitation within the non-absorbing region. Our analysis, using theoretical models and *ab-initio* quantum chemical computations, demonstrates that this phenomenon is due to an initial-state preparation effect of direct photoexcitation from the ground state singlet to excited triplet states. The direct photoexcitation leads to similar triplet-state populations for both optical excitation regions. Due to low intersystem crossing rates from the excited singlet states, these initial triplet populations determine the intensities of the EPR spectra [1].

The other part of the thesis focuses on the design of organic π-stacked molecular bridges that enable coherent TET over long-distances. We propose design principles for optimizing the speed of bridge-mediated TET. These design rules imply low inner-sphere exciton reorganization energies, low static and dynamic disorder and enhanced π-stacking interactions between nearest-neighbour chromophores. These features lead to triplet-exciton eigenstates that are delocalized over several units even at room temperature. We propose various molecular structures that satisfy these criteria and that can be used as bridging wires linking triplet donors to acceptors. We perform *ab-initio* electronic-structure computations, molecular-dynamics simulations and density-matrix simulations that predict fast TET along the proposed molecular bridges, with effective intra-bridge TET rates of the order of 0.1 psec for bridge lengths of up to 50 chromophore units [2].

1) Mavrommati, S. A.; Skourtis, S. S. *J. Chem. Phys.* **2020**, *152*, 044304.
2) Mavrommati, S. A.; Skourtis, S. S. *J. Phys. Chem. Lett.* **2022**, *13*, 9679-9687.