



Πανεπιστήμιο
Κύπρου

ΤΜΗΜΑ ΦΥΣΙΚΗΣ

Το Τμήμα Φυσικής του Πανεπιστημίου Κύπρου
σας προσκαλεί την

Δευτέρα, 20 Δεκεμβρίου 2021, ώρα 10:00
στην αίθουσα B228, στο κτίριο 13 στην Πανεπιστημιούπολη

στην παρουσίαση της Διδακτορικής Διατριβής της Στέφανης Βαλιαντή

“Molecular Charge-transfer and Excitonic Processes: from Bridge-mediated Electron Transfer and Transport to Bridge-mediated Singlet Fission”

This Ph.D. thesis describes research work on molecular electron transfer (ET) and transport (ETr), and on molecular Singlet Fission (SF) processes. The underlying objective of the research is to develop a physical understanding of how to control ET-ETr and SF in molecules by modifying the molecular structure.

Molecular junctions are ideal systems for the investigation of ETr mechanisms. We describe theoretical modelling of ETr in hybrid metal – ET protein - metal heterojunctions, focusing on a large set of experimental results that measure the current-voltage and current-temperature behavior of the junctions. Our analysis identifies the ETr mechanisms that are compatible with the experimental results. In addition, using analytical modelling, we propose a D-B-A molecular junction architecture, functioning in the incoherent hopping regime, that is suited for establishing direct correlations between the electrode-to-electrode current and the intra-molecular D-to-A ET rate. Thus, the Marcus inverted regime, observed in solution-phase ET, can now be probed in a completely different environment through the current, by varying the bias in a molecular junction.

The other part of the thesis focuses on the investigation of SF rates in molecular D-B-A systems. The main goal is to understand how a bridge linker connecting D and A can tune the effective SF coupling that leads to D-A-separated correlated triplets. For this purpose, we develop an analytical/computational framework to explore structure-function relationships for SF in D-B-A molecular architectures. This semi-analytical approach, based on Configuration Interaction Singles/Doubles theory, is also used to explain the recently-observed bridge-resonance effect and to guide computational and experimental searches for D-B-A systems with tuned SF rates.

Η παρουσίαση θα είναι ανοικτή στο κοινό μέσω τηλεδιάσκεψης:

<https://ucy.zoom.us/meeting/register/tJAld-yvrzqGt2pSKBbzL06gs0I5M4WjAKH>

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