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ΔΙΑΛΕΞΗ

"Theoretical assistance in designing Photoinduced Electron Transfer and Intramolecular ChargeTransfer systems"

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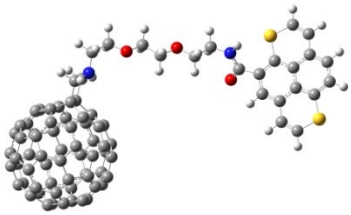
Αίθουσα σεμιναρίων στο ισόγειο του ΕΙΕ

Abstract



The selective recognition of molecules, the design of bio-mimetic systems of photosynthesis, the design of photonic molecular electronic devices for controlling the emission of light and many other applications have as key process the charge transfer mechanism. A great deal of effort internationally has been devoted to the goal of obtaining fundamental information at the molecular level. The biggest obstacles for the reliable treatment of such systems, stem from the large size of these systems that hinders the rigorous treatment of the excited states, which is required for comprehension of the charge and energy transfer mechanisms even at the simplest levels.

In this presentation, instead of solving the charge transfer problem rigorously, we are trying to handle it using simple existing theoretical methods, and physical insight. In this manner information is obtained which may be of assistance to experimental attempts.

Two approaches will be described:

(1) molecular orbital (MO) energy level diagrams , configuration interaction (CI) concepts and potential energy surfaces are used to predict/rationalize the possibility of charge transfer and energy transfer in a donor-acceptor system.

(2) calculated or experimental values for Ionization Potential (IP), Electron Affinity (EA) and excitation energies, along with estimation of the electron-hole Coulomb interaction energy are used to describe the energetics of charge-transfer processes in different systems.