Quantum photoelectrochemistry of nanoscale solar energy conversion processes

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Quantum photoelectrochemical calculations of key properties that include excited state properties, interfacial electronic interactions in general, and long-range charge separation via photoinduced heterogeneous electron transfer processes in particular, are made on a range of nanoscale solar energy conversion systems using first principles calculations.[1]

Emerging capabilities to theoretically investigate excited state evolution in light-harvesting metal complexes beyond the Franck-Condon region are explored through calculations of manifolds of multidimensional potential energy surfaces (Figure 1a).[2]

DFT and TD-DFT calculations of promising donor-acceptor (D-A) polymers for bulk heterojunction solar cells provide evidence for opportunities to achieve enhanced optical and electronic properties by utilizing side-group stacking strategies to facilitate increased intra-chain structural ordering (Figure 1b).[3]

Interfacial electronic interactions in dye-semiconductor interfaces provides continued challenges in terms of prospects to achieve improved functional control of intrinsically disordered interfaces using new sensitization strategies, e.g. employing ruthenium star complexes, that promote control of long-range interfacial electron transfer in a spacer-mediated weak coupling limit (Figure 1c).[4]

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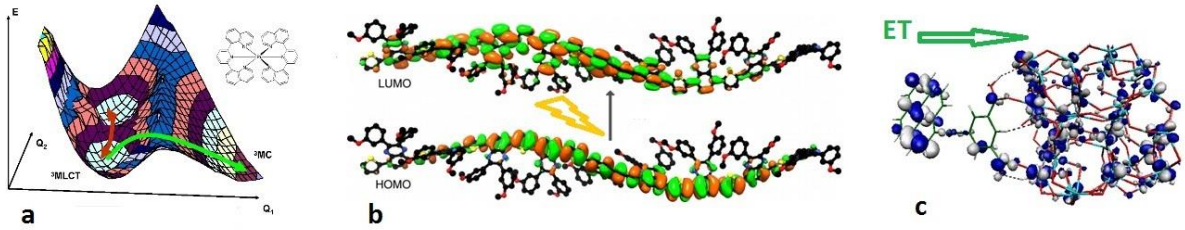

Figure 1. (a) Light-harvesting transition metal complex triplet PES, (b) D-A polymer excitation, (c) dye-sensitized nano-TiO_2 interface.