

Electrochemical and Photochemical Behavior of Novel Fullerene-Based Supramolecular Systems

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Recent studies have demonstrated that the fullerenes behave as excellent electron acceptors and good energy traps useful for constructing artificial photosynthetic systems. In this regard, model systems, both covalently linked and self-assembled, have revealed rich electrochemistry corresponding to the different redox-active entities and interesting photochemistry originating from them. Such studies have also shown that fullerene bearing donor-acceptor

supramolecules could be potential candidates to construct photovoltaic devices.

In the present contribution, we summarize results on our newly developed covalently as well as self-assembled fullerene bearing supramolecular systems. The covalently linked dyads and triads utilized porphyrin, ferrocene, tetrathiafulvalene as donors while fullerene and dinitrobenzene as acceptors. The electrochemical behavior of the different redox active entities bearing dyads and triads has been investigated and modeled by using *ab initio* B3LYP/3-21G* methods. The calculated HOMO and LUMO's track the observed site of electron transfer of the supramolecular entities. Multiple modes of binding has been introduced to form stable porphyrin-fullerene conjugates with defined distance and orientation. Both steady-state and time-resolved emission studies revealed efficient charge separation and charge recombination in the studied covalently as well as self-assembled supramolecular systems.