 ICCES, vol.19, no.4, pp.127-127

Towards computational design of Fe(II) chromophores for solar energy conversion

Elena Jakubikova, David N. Bowman

Summary

The Sun is an abundant source of energy capable of meeting all our energy needs if properly harvested. Some of the ways to utilize solar energy is conversion of sunlight to electricity via photovoltaic solar cells or to chemical fuels via photocatalytic synthetic cells. Many of such systems are designed around a photoactive molecule (a chromophore) anchored to a semiconductor. The conversion of sunlight to electricity occurs via absorption of light by the chromophore, followed by the interfacial electron transfer between the chromophore and semiconductor. We investigate the use of Fe(II)-polypyridine compounds as chromophores in the molecular assemblies for solar energy conversion. The molecular systems considered are relatively large (50 atoms or larger) and are most amenable to calculations using the density functional theory. Calculations of ground and excited state properties of Fe(II) complexes pose some interesting challenges for theory, due to the existence of low-lying excited states and open shell ground states. The results obtained lead us to better understanding of the structure-property relationships in these complexes and have implications for development of novel chromophores for solar energy conversion applications.