Materials Seminar

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Molecular and Material Approaches for Solar Energy Conversion and Storage

Realizing the scalable, cost-effective conversion of solar energy to electricity and chemical fuels is the biggest scientific challenge of our time. This talk will describe our efforts to understand and control the processes determining the efficiency of promising solar energy conversion systems based on nanoscopic metal oxide materials. One particularly interesting system is the dye-sensitized solar cell, DSSC, where the performance depends on the interplay of various electron-transfer reactions between molecular chromophores, mesoporous metal oxide photoelectrodes and redox shuttles dissolved in solution. Detailed understanding of some of the key processes, such as recombination, have been thwarted by lack of methods to accurately determine the energetics of the semiconductor (donor) and control over redox shuttle (acceptor) properties. Spectroelectrochemical methods will be presented that simultaneously produce the conduction band energy and the extinction coefficient of free electrons in nanoparticle TiO_2 electrodes. In addition, this methodology allows accurate quantification of the trap state distribution and band unpinning. A series of cobalt complexes, where ligands modulate the electron-transfer self-exchange rate constant by nine orders of magnitude via spin state variations, were employed as redox shuttles in DSSCs. Application of Marcus theory with knowledge of the semiconductor energetics allow the differences in self-exchange rate constants to quantitatively account for differences in regeneration efficiency and electron diffusion length – which is a function of recombination – of the redox shuttles measured. These results point to a new energy and kinetic space of redox shuttle which have the capability of achieving high efficiencies in next-generation DSSCs, which will be discussed. Nanostructured hematite (α-Fe_2O_3) comprises another system of interest for photoelectrochemical (PEC) water splitting due to its unique combination of suitable optical and electrochemical properties combined with excellent stability and elemental abundance. We have utilized PEC and impedance spectroscopy measurements to show the accumulation of holes in surface states of hematite, which can recombine with conduction band electrons, controls the water oxidation onset potential and thus water splitting efficiency.

Monday, September 19

3:30 pm in room 1315