Porosity Effects in the Design of Nanocrystalline Dye Sensitized Solar Cells

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The present analysis of dye sensitized semiconductors is pursued through an examination of the classical aspects of the discipline of chemistry: energetics, dynamics, and structure. Theory and experiment have come together in the literature to provide a picture of the rudimentary requirements for an efficient spectral sensitization of solids.[1,2]

In light of the commercial potential of dye sensitized solids as a nanocrystalline, dye-sensitized solar cell, these principles have been utilized in the attempt to design a better and more efficient solar cell than the Ru-based nanocrystalline TiO_2 cell first presented more than a decade ago.[3] Even though new materials and systems have been developed, however, none has yet exceeded the long term performance of the Ru/TiO₂ system.

In this work I present a perspective on nanocrystalline dye sensitized solar cells that is based not on these fundamental principles, but rather on porosity concepts that allow a different viewpoint to be taken on the design of these cells. The discussion is highlighted by work from the literature and recent experimental results from our laboratory.

The porosity characteristics of the nanocrystalline solar cell have a defining impact in several areas. The first is in the conductive porosity for charge flow through the device. The second is the dielectric inhomogeneity induced by the porosity. This impacts the interfacial charge transfer, separation, and recombination. The last is the optical scattering of incident light caused by largesized particles in the nanocrystalline matrix as well as by the statistical clusters of sintering defects in the nanocrystalline solid structure

The first effect of porosity involves the conductance of the two complementary pathways of the nanocrystalline system: charge transport through the regenerating system to the sensitizer and electron transport through the nanocrystalline solid to the collector electrode. Literature studies of this problem have focused on overall current flow, but do not examine the statistical problem of porosity–induced sink and source sites of charge.[4,5]

The dielectric heterogeneity of nanocrystalline systems is further increased by an increase in porosity. Statistically, the average dielectric constant about a sensitizing dye is determine by a weighted mean of the dielectric environment. This affects electron transfer at surfaces through the rearrangement energy of the molecules involved, the sensitizing dyes and the regenerating agent; detailed examination of the problem involves a microscopic description of the dielectric environment.[6] This factor is further affected by the structure of the dye molecule, since the low dielectric constant of the organic materials differs greatly from that of the solid and regenerating electrolyte solutions. Statistical evaluations of these effects have been made and will be presented along with experimental data from cells made with novel sensitizing dyes.

Last, the scattering of light by the nanocrystalline structure will be examined. Although one may induce this scattering intentionally through the use of large particles of conductive solid, this process also occurs through a statistical graininess induced by non-dispersed colloids of the solid.

The result of each of these porosity considerations is a statistical distribution of current sinks and sources and optical hot spots that overlay each other within a nanocrystalline layer. The product of these play a role in defining the performance of a dye-sensitized solar cell.

References:

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