ELECTRONIC STRUCTURE OF DYE-SENSITIZED SOLAR CELL INTERFACES

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Dye-sensitized solar cell structures were deposited in vacuum directly from solution, and their orbital/valence bands line-ups were determined using photoemission spectroscopy. This was achieved by first depositing TiO_2 nanoparticles on indium tin oxide (ITO) substrates, and then injecting a coating layer of $RuL_2(NCS)_2$ [cis-bis(4,4'-dicarboxy-2,2'-bipyridine)–bis(isothio-cyanato)-ruthenium(II)] ("N719", a prototypical dye used in many currently pursued device structures) dye. Both TiO_2 and N719 films were built up in several steps using electrospray. Electrospray enables the fabrication of clean, essentially uncontaminated thin films of organic molecules and nanoparticles directly in vacuum. (Fig.1 shows a scanning electron microscopy image of a completed interface structure-the morphology is comparable to TiO_2 thin films fabricated with methods used for device fabrication). After each deposition step characterization by x-ray and ultraviolet photoemission spectroscopy (XPS, UPS) was performed. The resulting sequence of spectra allowed the determination of charge injection barriers and interface dipoles at the ITO/TiO_2 and TiO_2/N3 interfaces. While the presented data confirm that the TiO_2/dye interface electronic structure is conducive to exciton separation, they also suggest that the interface between TiO_2 and ITO may pose a significant barrier to electron injection into the ITO electrode. Fig.2 shows the electronic structure of the interface as determined on a sputtered ITO substrate.

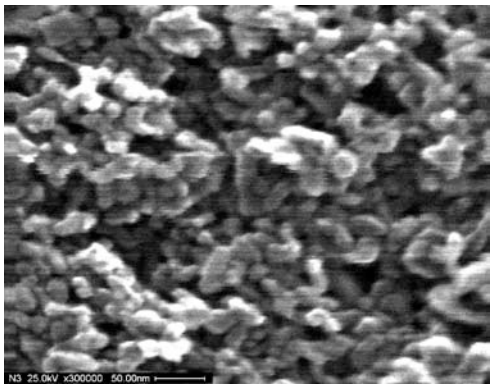

Fig.1: SEM image of TiO_2/dye interface as prepared by electrospray injection in vacuum.

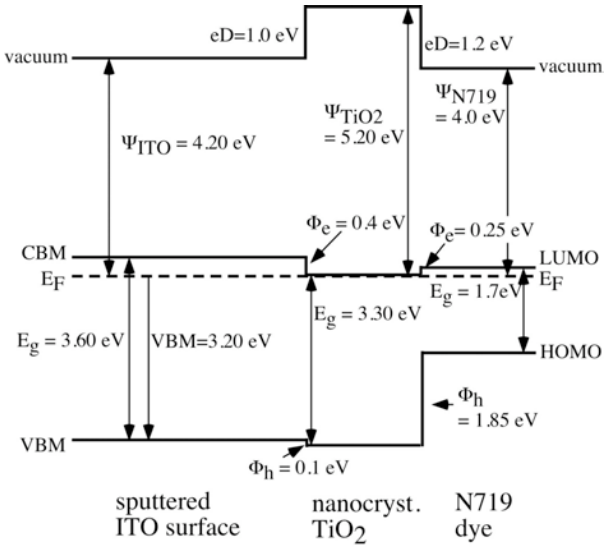

Fig.2: Electronic structure of ITO/TiO_2/dye (N719) interface as determined from XPS and UPS measurements.