Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

**Influence of the Sensitizer Protonation and Adsorption Mode on the Efficiency of Dye-sensitized solar cells** ANNABELLA SELLONI, Princeton University, FILIPPO DE ANGELIS, SIMONA FANTACCI, Universita' di Perugia, Italy, MOAMMHED NAZERUDDIN, MICHAEL GRAETZEL, Swiss Federal Institute of Technology, Lausanne, Switzerland — Dye sensitized solar cells (DSSCs) represent a promising approach to the direct conversion of light into electrical energy at low cost and with high efficiency. In these devices, a dye sensitizer absorbs the solar radiation and transfers the photoexcited electron to a nanostructured TiO2 electrode. We have studied the electronic structure of different Ru(II)-polypyridyl dyes adsorbed onto a model TiO2 nanoparticle by means of first principles Density Functional Theory calculations. Our results suggest that two different electron injection mechanisms (adiabatic and non-adiabatic) may be present in DSSCs employing dyes carrying a different number of protons. We also found that sensitizers with inequivalent bipyridine ligands exert strong dipolar fields at the TiO2 surface, causing a conduction band down-shift and a reduction of the cell open circuit potential, thus resulting in a reduced DSSC efficiency.

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Date submitted: 25 Nov 2007 Electronic form version 1.4