Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

TiO2 nanowire sensitized by organic dyes for photovoltaic applications: influence of binding groups and molecular dimension[1] SHENG MENG, EFTHIMIOS KAXIRAS, Harvard University Physics Department — We investigate the electronic couplings including charge separation, injection, and recombination processes between a TiO2 nanowire and a set of organic dye sensitizers, based on the full time-dependent density functional theory treatment of electron excitation and atomic vibrations. For all the cases the highest occupied molecular orbital (HOMO) of dye molecules are found being located in the middle of the TiO2 bandgap and the lowest-unoccupied molecular orbital (LUMO) close to the TiO2 conduction band minimum, leading to enhanced visible light absorption and ultrafast electron injection into the TiO2 conduction band. The influences of the anchoring groups and molecular dimensions to the dye injection dynamics and electron-hole recombination process are discussed.

[1]This work was supported in part by DOE CMSN Grant DE-FG02-05ER46226 and the Harvard University Center for the Environment.

Sheng Meng
Harvard University Physics Department

Date submitted: 21 Nov 2008 Electronic form version 1.4