Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

First principles modeling of panchromatic dyes for solar cells applications. ROSA DI FELICE, ARRIGO CALZOLARI, Centro S3, CNR Istituto di Nanoscienze, Modena, Italy, RUI DONG, North Carolina State University, MARCO BUONGIORNO NARDELLI, University of North Texas — The state-of-the-art dye in Grätzel solar cells, N719, exhibits a total solar-to-electric conversion efficiency of 11.2%. However, it severely lacks absorption in the red and the near infrared regions of the electromagnetic spectrum, which represent more than 70% of the solar radiation spectrum. Using calculations from first principles in the time-dependent domain, we have studied the electronic and optical response of a novel class of panchromatic sensitizers that can harvest solar energy efficiently across the visible and near infrared regions, which have been recently synthesized [A. El-Shafei, M. Hussain, A. Atiq, A. Islam, and L. Han, J. Mater. Chem. **22**, 24048 (2012)]. Our calculations show that, by tuning the properties of antenna groups, one can achieve a substantial improvement of the optical properties.

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Date submitted: 28 Nov 2012 Electronic form version 1.4