Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Ab initio calculation of the excited state properties of spiropyran

EMMANOUIL KIOUPAKIS[1], STEVEN G. LOUIE, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — The photochromism of spiropyran/merocyanine molecules has been the subject of many experimental and theoretical studies. However, several questions remain open, in particular the excited state dynamics and the role of the triplet state. In this work, we use ab initio techniques based on Density Functional Theory and Green's functions methods based on the GW approximation to the electron self energy and Bethe-Salpeter equations to study the ground and excited states of spiropyran/merocyanine for various geometries. Our results are compared with previous work. This work was supported by National Science Foundation Grant No. DMR07-05941, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NERSC and TeraGrid resources provided by SDSC and Indiana University.

[1]Fellow of the "Alexander S. Onassis" Foundation

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Date submitted: 01 Dec 2007 Electronic form version 1.4