MAR13-2012-020151

Abstract for an Invited Paper
for the MAR13 Meeting of
the American Physical Society

Computational spectroscopy using many-body perturbation theory: Large scale calculations without virtual orbitals[1]

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An accurate description of electronic excitations is essential to model and understand the properties of several materials of fundamental and technological interest. First principles, many-body techniques based on Green's functions are promising approaches that can provide an accurate description of excited state properties; however their applicability has long been hindered by their numerical complexity. In this talk we will summarize some recent methodological developments based on many-body perturbation theory for the efficient calculation of optical absorption spectra [1], photoemission spectra [2], and multiple exciton generation rates [3]. Several applications to realistic materials will be presented, with emphasis on materials for solar energy applications; these include silicon nanowires and bulk tungsten oxide, that are promising photoelectrode materials in water splitting solar cells, molecules used in organic photovoltaics, and semiconductor nanoparticles with potential use in third generation photovoltaic cells based on multiple exciton generation. Work done in collaboration with Y. Ping, T. A. Pham, M. Voros, D. Lu, H.-V. Nguyen, S. Wippermann, A. Gali, G. T. Zimanyi, and G. Galli.

*Present address

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[2] H.-V. Nguyen, T.A. Pham, D. Rocca, G. Galli, Phys. Rev. B 85, 081101 (2012).
[3] M. Voros, D. Rocca, G. Galli, G.T. Zimanyi, A. Gali, submitted (2012).

[1]Work supported by NSF-CHE-0802907.