GW and BSE

We compute transport and optical properties using many-body perturbation theory within the GW approximation and the Bethe-Salpeter Equation for systems where standard-DFT approaches fail, like organic molecules and their crystals. For such systems, standard approximations to DFT exchange-correlation energy are not sufficient because of self-interaction and derivative discontinuity errors, and the lack of non-locality in the approximate exchange-correlation functional. In these cases, we obtain addition/removal energies as a first order correction to a mean-field starting point (typically DFT), and optical excitation energies by solution of the bethe-salpeter approach, as implemented by Rohlfing and Louie. We use the BerkeleyGW code developed by collaborators at UC Berkeley, and also the GW implementation in VASP.

Optical properties of pentacene and PTCDA

Alison Hatt posted on Mar 29, 2012
As prototypical organic systems, pentacene and PTCDA are central to the growing field of molecular-scale science, yet their electronic and optical properties are not well understood. Applying the tools of many-body perturbation theory to these systems, we study charge transport and optical absorption, and probe the nature of optically generated excitons.

Related Publications

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M. J. van Setten, F. Caruso, S. Sharifzadeh, X. Ren, M. Scheffler, F. Liu, J. Lischner, L. Lin, J. R. Deslippe, S. G. Louie, C. Yang, F. Weigend, J. B. Neaton, F. Evers, and P. Rinke, "$\text{GH}\text{100}: \text{Benchmarking} \ G_0\ W_0 \ \text{for \ molecular \ systems}," \text{J. Chem. Theory Comput. 11,} 5665 (2015). Abstract

Florian Brown-Altvater posted on Feb 02, 2015

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