Combining density-functional theory and many-body methods

Julien Toulouse

Laboratoire de Chimie Théorique, Université Pierre et Marie Curie, CNRS, Sorbonne Universités

Paris, France

Nowadays, a major strategy for improving approximations in density-functional theory (DFT) is to combine DFT with many-body methods such as many-body perturbation theory. Range separation of the electron-electron interaction provides a practical way of performing such a combination by using a (semi)local-density approximation for the short-range part and an explicit many-body approximation for the long-range part. It combines the best of both worlds: an accurate and compact description of short-range interactions by DFT approximations and an accurate description of long-range nonlocal interactions by many-body approximations, while avoiding any double counting of electron correlations.

After giving an overview of such approaches, I will present some recent advances concerning:

- Range-separated hybrid methods for describing ground-state correlations in molecular and solid-state systems, based on second-order perturbation theory and random-phase approximations[1,2];

- Range-separated hybrid methods for calculating excitation energies in molecular systems, based a long-range frequency-dependent second-order Bethe-Salpeter correlation kernel[3].

[1] B. Mussard, P. Reinhardt, J. G. Ángyán, J. Toulouse, J. Chem. Phys. **142**, 154123 (2015).

[2] G. Sansone, B. Civalleri, D. Usvyat, J. Toulouse, K. Sharkas, L. Maschio, J. Chem. Phys. **143**, 102811 (2015).

[3] E. Rebolini, J. Toulouse, J. Chem. Phys. **144**, 094107 (2016).