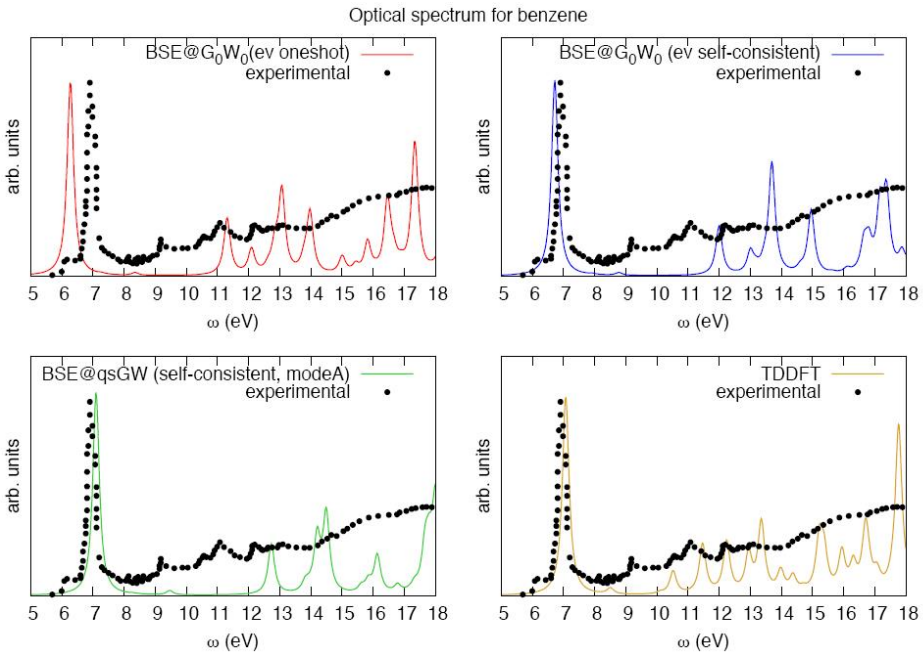
# Optical spectra and quasiparticle energies of molecules using a local basis

**Mathias P. Ljungberg,** Peter Koval, Francesco Ferrari, Dietrich Foerster and Daniel Sánchez-Portal

DIPC (Donostia International Physics Center)
Paseo Manuel de Lardizabal, 4
20018 Donostia-San Sebastián (Gipuzkoa), Spain

mathias.ljungberg@gmail.com

The Bethe-Salpeter equation (BSE) is the state of the art for computing optical spectra for solids and molecular clusters. Here we present an implementation of BSE for clusters that scales asymptotically like O(N^3) with the number of atoms, achieved by exploiting the locality of the problem in the local basis set representation and by using the Haydock recursion method to compute the spectrum. Using a pseudhermitian Lanczos algorithm we can go beyond the Tamm-Dancoff approximation within our iterative scheme. As a starting point for the BSE we compute quasiparticle energies with our low-scaling GW implementation [1], retaining the frequency dependence of all quantities and thus avoiding the plasmon-pole model or similar schemes. The initial wave functions are taken from a preceding SIESTA calculation. We discuss the influence of self-consistency on the quasiparticle energies [2] and its effect on the BSE spectra. We also investigate the satellite peaks that are present in the GW density of states. Computed GW/BSE spectra are shown for some organic molecules of medium size that are relevant for photovoltaic applications.




## References

[1] D. Foerster et al. J. Chem. Phys. 135 (2011) 074105.
[2] P. Koval et al. Phys. Rev. B 89 (2014) 155417.