On the accuracy of BSE/*GW* properties: dipole moments and geometries

DENIS JACQUEMIN[1,2]

[1]*Nantes Université, CNRS, CEISAM UMR 6230, Nantes F-44000, France*
[2]*Institut Universitaire de France (IUF), Paris F-75005, France*
Denis.Jacquemin@univ-nantes.fr

ABSTRACT

The many-body Green's function Bethe−Salpeter equation (BSE) formalism has become increasingly popular in molecular chemistry for evaluating excited-state energies and related oscillator strengths. However, less is known about the performances of this formalism for other excited-state properties. In this contribution, I will summarize our recent efforts aiming at establishing the *pros* and *cons* of BSE/*GW*, with respect to both TD-DFT and CC2, in the framework of the determination of excited-state dipoles [1,2] and potential energy surfaces [3].

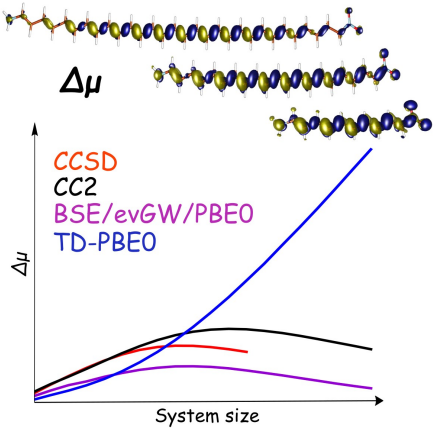

Figure 1: Evolution with size of the excess dipole in push-pull chains

References

[1] Knysh, I.; Villalobos-Casto, J.; Duchemin, I.; Blase, X.; Jacquemin D. Exploring Bethe−Salpeter Excited-State Dipoles: The Challenging Case of Increasingly Long Push−Pull Oligomers. *J. Phys. Chem. Lett.* **2023**, *14*, 3727.

[2] Knysh, I.; Villalobos-Casto, J.; Duchemin, I.; Blase, X.; Jacquemin D. Excess and Excited-State Dipole Moments of Real-Life Dyes: A Comparison Between Wave-Function, BSE/*GW*, and TD-DFT Values. *Phys. Chem. Chem. Phys*. **2023**, *25*, 2993

[3] Knysh, I.; Duchemin, I.; Blase, X.; Jacquemin D. Modelling Excited State Potential Energy Surfaces with Bethe-Salpeter Equation Formalism: The 4-(Dimethylamino)Benzonitrile Twist. *J. Chem. Phys*. **2022**, *157*, 194102.