Koopmans-Compliant Functionals and Bethe-Salpeter Equation for Spectroscopy Simulations

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In this talk, I introduce the theoretical formulation and the practical implementation of Koopmans-compliant (KC) functionals [1], which are constructed to enforce piecewise linearity in energy functionals with respect to fractional occupations (i.e., with respect to charged excitation); their accuracy has been shown via not only simulating molecular photoemission spectra in excellent agreement with experimental ultraviolet photoemission spectroscopy but also accurately predicting band gaps and band structures of the crystal semiconductors [2,3]. In particular, I discuss how to combine these functionals with the solution of the Bethe-Salpeter equation via the calculation of the screened Coulomb interaction in a finite field method [4] to compute optical spectra and exciton binding energies of molecules and solids. This approach does not consider explicit evaluation of dielectric matrices nor of virtual electronic states and is easily applied to large systems. I report its applications to predict the exciton binding energies of several molecules and simulate the absorption spectra of condensed systems of sufficiently large sizes, including water and ice samples with hundreds of atoms.

References:

[1] G Borghi et al PRB 90, 075135 (2014)
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[3] NL Nguyen, et al. Physical Review X 8, 021051 (2018)
[4] NL. Nguyen, et al. PRL **122**, 237402 (2019)