Contribution ID: **242** Type: **Poster**

Changes in polarization dictate necessary approximations for modeling electronic de-excitation intensity: an application to X-ray emission

We systematically investigate the underlying relations among different levels of approximation for simulating electronic de-excitations, with a focus on modeling X-ray emission spectroscopy (XES). Using Fermi's golden rule and explicit modeling of the initial, core-excited state and the final, valence-hole state, we show that XES can be accurately modeled by using orbital optimization for the various final states within a Slater-determinant framework. However, in this paper, we introduce a much cheaper approach reliant only on a single self-consistent field for all the final states, and show that it is typically sufficient. Further approximations reveal that these fundamentally many-body transitions can be reasonably approximated by projections of ground state orbitals, but that the ground state alone is insufficient. Furthermore, except in cases where the core-ionization induces negligible changes in polarization, linear-response approaches within the adiabatic approximation will have difficulty in accurately modeling de-excitation to the core level. Therefore, change in the net dipole moment of the valence electrons can serve as a metric for the validity of the linear-response approximation.

Topic

Theory

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Session Classification: Poster session