

Title: Coupled-cluster theory for condensed-phase spectroscopy

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Abstract:

Wave function-based quantum chemistry techniques, such as MP2 and coupled-cluster theory, are starting to be applied to condensed-phase materials, leading to accurate and controlled treatments of electron correlation. I will describe the first applications of excited-state coupled-cluster theory (so-called equation-of-motion coupled-cluster) to systems with explicit periodicity. This approach represents a departure from time-dependent diagrammatic Green's function techniques like the GW approximation. In particular, I will present results for the spectral function of the paradigmatic uniform electron gas, where equation-of-motion coupled-cluster theory correctly produces satellite structure due to electron-plasmon coupling and yields a quasiparticle bandwidth in good agreement with experimental photoemission data; these results are compared with those obtained from the GW and GW+cumulant approximations. I will also present results for the quasiparticle band structure and band gaps of fully atomistic solids such as diamond and silicon. Both formal and computational aspects of the approach, including the relation to the GW approximation, will be discussed.