The richness of excitations in model and real materials: linear response TDDFT

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In the framework of linear response time-dependent density functional theory (LRTDDFT), the exact exchange-correlation (xc) kernel $f_{xc}(q, \omega)$ determines the groundstate energy, excited-state energies, lifetimes, and the time-dependent linear density response of any homogeneous many-electron system. The recently developed dynamic MCP07 exchange-correlation kernel delivers excellent-quality correlation energies for the ground state, predicting a static charge density wave (CDW) at low density, and plausible finite plasmon lifetimes at all wavevectors in the homogeneous electron gas (HEG) model (this latter feature for the first time within TDDFT [1-3]).
The dielectric function in principle can encompass xc effects through the MCP07 or other kernels that are relevant to describe rich phenomena of the low-density physics in the HEG. Beside collective plasmon excitations, the dielectric function can reveal collective electron-hole excitations, often dubbed “ghost excitons” [4].
But real quantum materials have even more complexity than the HEG. Bulk and monolayer $TiSe_2$ are known as CDW materials which can be driven by excitonic insulator or electron-phonon coupling mechanisms. This complexity requires simultaneous accuracy for both ground and excited states.
My talk will give details of work done with xc kernels in model HEG system, and it will discuss more details about the extension of the applicability of ground state DFT and LR-TDDFT to excitations in real quantum materials exemplified by$TiSe_2$ [5].

References

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