Wave function based correlation in solids: RPA and beyond

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During the last few years, we have been working on a wave function based treatment of electronic correlation in solid state systems. We have implemented the evaluation of electronic correlation by means of the Adiabatic-Connection-Fluctuation-Dissipation-Theorem as well as Coupled-Cluster Doubles theory in the Random-Phase-Approximation (ACFDT-RPA [1], drCCD [2]), within the projector-augmented-wave [3] code VASP.
I will characterize the accuracy of the RPA with respect to the description of lattice constants, bulk moduli, and atomization energies of several archetypical solid state systems. Furthermore I will present results on the CO adsorption on metallic surfaces within the RPA.
Additionally, I will discuss recent work on the socalled RPA + 2^{nd}-order *screened* exchange (SOSEX), a method that goes beyond the RPA and exactly eliminates self-correlation for one and two-electron systems [4].

References

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