Accurate Ground-state Correlation Energies Within the RPA and Beyond: From Theory to Realistic Applications

Dario Rocca

LPCT Laboratory

University of Lorraine and CNRS, Nancy (France)

Email: dario.rocca@univ-lorraine.fr

Abstract:
Despite the high computational cost the adiabatic connection fluctuation dissipation theorem (ACFDT) represents a promising approach to improve the description of the electronic correlation within density functional theory. The simplest approximation that can be applied in the context of the ACFDT is the random phase approximation (RPA). First, I will show that the RPA correlation energy can be efficiently computed within a periodic plane-wave implementation by using dielectric eigenpotentials as a compact auxiliary basis set and the Lanczos algorithm. Then, within a similar numerical framework I will demonstrate that the accuracy of the RPA can be significantly improved by introducing a kernel containing an approximate electron-hole exchange term. Finally, by using perturbation theory the ACFDT approximations will be combined with molecular dynamics simulations to obtain accurate finite-temperature properties. A series of applications of these methodologies will be presented throughout, including the calculation of a prototypical molecular enthalpy of adsorption in zeolite (CH_4 on protonated chabazite at 300 K).