Time-Dependent Density-Functional-Theory from a Practitioners Perspective

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The talk gives a brief summary of applications of time-dependent density-functional theory to metal clusters. More specifically, density-functional theory is employed at the level of the time-dependent local-density approximation (TDLDA). The theoretical part presents the basics of TDLDA, discusses tests of applicability, and addresses the Vlasov-LDA as semi-classical limit of TDLDA which is particularly suited for violent excitations. After a brief overview over the typical features of clusters (scales of times, lengths and forces), a guided tour through selected applications will be given. This embraces dynamics in the linear regime (optical response), coupling of electronic and ionic motion, and goes up to violent non-linear processes.

Pure TDLDA becomes insufficient in the regime of high excitations. Dynamical correlations through electron-electron collisions have to be added. A practical and well tested scheme exists within the semi-classical approach extending Vlasov-LDA to the Vlasov-Uehling-Uhlenbeck (VUU) scheme. The effect from electron-electron dissipation will be demonstrated on recent VUU results. As an open end, first steps towards a fully quantal treatment of electron-electron collisions will be sketched. The approach is based on TDLDA complemented by occasional stochastic jumps amongst neighboring TDLDA trajectories.