Benchmarking Gaussian Basis sets for LASER-driven molecular properties and Electrostatics-based search of minimum energy metal clusters

Thesis Abstract

Electronic-responses of molecules interacting with high intensity linearly polarized light are studied and analysed for multi-electron systems. These electronic-responses are simulated using an in-house code, for real-time Hartree-Fock (RTHF) method, which solves the time dependent Schrödinger equation using the (t,t′)-method. The time-dependent properties (Norm, induced dipole etc.) are simulated using RTHF-method. The effect of increasing laser-field strength on the electronic-dynamics is also presented. In particular, certain prototypical systems have been chosen to benchmark and understand the usage of standard Gaussian basis sets in the electronic dynamics at a fixed nuclear geometry,Similarly, the effect of linearly polarized laser-pulse is studied for linearly conjugated molecules. In the second part of the thesis, an application of Molecular Electrostatic Potential (MESP) is discussed for the case of metal clusters. This electrostatic binding method (EBM) is tested for locating minimum energy isomers of silver clusters (Ag_n), up to n = 20, at four different levels of theories.