Implementation of the core-valence separation technique within the local CC2 linear response model for calculating the x-ray absorption spectra of large molecules

Ernst-Christian Flach[1], Martin Schütz[1], Denis Usvyat[1]

[1]Humboldt-Universität zu Berlin, Germany

Ernst-Christian.Flach@hu-berlin.de

Abstract

Using conventional methods, a large number of excited states would have to be calculated in order to obtain x-ray absorption spectra. The core-valence-separation (CVS) ansatz avoids this issue by neglecting all contributions of the valence electrons while solving the fundamental eigenvalue problem. The CVS ansatz was implemented for the local CC2 model that can be applied to extented systems.

Keywords

local correlation methods, coupled cluster, x-ray absorption spectra