Implementing real-time propagation time-dependent density functional theory for computing electronic circular dichroism spectra of Ag clusters

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DNA-stabilized silver clusters (Ag:DNA) and ligand-protected silver (LPAg) clusters have rapidly attracted interests due to their potential applications in wide range of nanotechnology, such as sensors and fluorescent imaging [1-2]. For these Ag clusters comparing experimental and computed electronic circular dichroism (ECD) spectroscopy is a very accurate indirect approach for probing structural properties, which are normally difficult to directly measure using X-ray techniques [3-5]. Accurate prediction of ECD spectrum for Ag:DNAs and LPAgs requires computing a large number of excited states. It may be prohibitively costly within the linear-response time-dependent density functional theory (LR-TDDFT) framework [5]. Here we represent an efficient method implemented in GPAW for computing entire ECD spectrum simultaneously based on real-time propagation time-dependent density functional theory (RT-TDDFT) and linear combination of atomic orbitals (LCAO) [6-7]. We also included some test cases here to show the accuracy and efficiency of our method.

References

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