Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Long-range corrected time-dependent density functional theory with spin-orbit couplings AYAKO NAKATA, TAKAO TSUNEDA, KIMIHIKO HIRAO, RIKEN, JST-CREST — Relativistic time-dependent density functional theory (TDDFT) is a powerful tool to include both of relativistic and correlation effects with low computational cost. However, TDDFT with conventional exchange functionals have severe problems in e.g. the reproducibility of charge transfer (CT) and Rydberg excitation energies and oscillator strengths. These problems are due to the lack of long-range exchange interactions in conventional exchange functionals. We have proposed long-range corrected (LC) DFT and have overcome these problems. Especially, LC-TDDFT succeeds in describing CT excitations with remarkable accuracy. CT excitations often play a major role in spin-forbidden transitions, because the spin-orbit couplings are significant for excitations inducing the changes in electron distributions. In this study, LC-DFT has been applied to a spin-orbit TDDFT to describe spin-forbidden transitions appropriately by TDDFT. Our results have demonstrated that LC-DFT accurately reproduces the splitting of ionization energies of heavy atoms and spin-forbidden excitation energies for which electrons are moved to widely-distributed orbitals.

Ayako Nakata
RIKEN, JST-CREST

Date submitted: 18 Nov 2010 Electronic form version 1.4