Contribution ID: **31** Type: **not specified**

Development of two-component relativistic time-dependent density functional theory for Molecular Properties

Wednesday, 21 June 2017 11:45 (30 minutes)

In this work, we have developed the two-component relativistic time-dependent density functional theory with spin–orbit interactions to calculate linear response properties and excitation energies. The approach is implemented in the NTChem program. The two-component relativistic TDDFT with spin–orbit interactions was successfully applied to the calculation of the frequency-dependent polarizabilities and the excitation spectra of several molecules containing heavy atoms.

Presenter: Prof. KAMIYA, Muneaki (Gifu University)