Contribution ID: **100** Type: **Poster**

Regularized relativistic corrections for polyelectronic and polyatomic systems with explicitly correlated Gaussians

Monday 10 June 2024 18:00 (2 hours)

Drachmann's regularization approach is implemented for floating explicitly correlated Gaussians (fECGs) and molecular systems. Earlier applications of Drachmannized relativistic corrections for molecular systems were hindered due to the unknown analytic matrix elements of $1/r_{ix}1/r_{jy}$-type operators with fECGs. In the present work, one of the $1/r$ factors is approximated by a linear combination of Gaussians, which results in calculable integrals. The numerical approach is found to be precise and robust over a range of molecular systems and nuclear configurations, and thus, it opens the route towards an automated evaluation of high-precision relativistic corrections over potential energy surfaces of polyatomic systems. Furthermore, the newly developed integration approach makes it possible to construct the matrix representation of the square of the electronic Hamiltonian relevant for energy lower-bound as well as time-dependent computations of molecular systems with a flexible and high-precision fECG basis representation.

Authors: RÁCSAI, Balázs (ELTE, Eötvös Loránd Tudományegyetem); Dr FERENC, Dávid (ELTE, Eötvös Loránd Tudományegyetem); Prof. MÁTYUS, Edit (ELTE, Eotvos Lorand University); MARGÓCSY, Ádám (ELTE, Eötvös Loránd Tudományegyetem, Budapest)

Presenter: RÁCSAI, Balázs (ELTE, Eötvös Loránd Tudományegyetem)

Session Classification: Poster Session 1