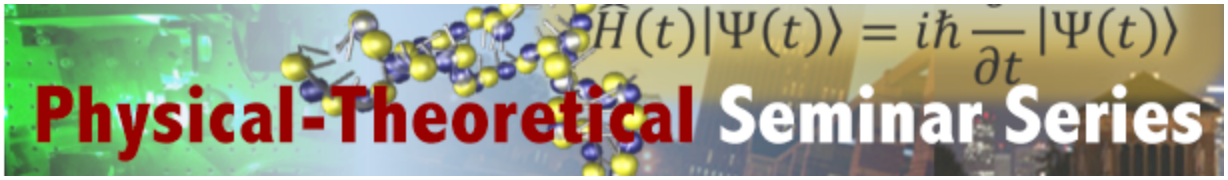

Monday, October 7, 2019, 12:00 pm
Zumberge Hall, ZHS 159

Professor Lan Cheng

Department of Chemistry
Johns Hopkins University

New advances in electronic structure methods with non-perturbative treatment of spin-orbit coupling

A new implementation of relativistic coupled-cluster (CC) methods using relativistic exact two-component Hamiltonian with atomic mean-field spin-orbit integrals (X2CAMF) is presented. The new implementation benefits from partial recovery of spin symmetry, hereby using atomic-orbital driven algorithms and exploiting the spin- free nature of instantaneous Coulomb interaction. This reduces storage requirements by an order of magnitude and thus significantly extends the applicability of relativistic CC methods. Applications deal with ground- and excited-state energies and properties for molecules containing early actinides, which are of significant interest to both actinide chemistry and atomic, molecular, and optical physics.

Suggested Reading:

1. A. Asthana, J. Liu, and L. Cheng, “Exact two-component equation-of-motion coupled-cluster singles and doubles method using atomic mean-field spin-orbit integrals”, *J. Chem. Phys.* **150**, 074102 (2019). https://doi.org/10.1063/1.5081715

2. J. Liu, L. Cheng, “An atomic mean-field spin-orbit approach within exact two-component theory for a non-perturbative treatment of spin-orbit”, *J. Chem. Phys*. **148**, 144108 (2018). https://doi.org/10.1063/1.5023750

Hosted by Professor Anna Krylov

The scientific community is invited

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