Scientific Achievement

Realized greater accuracy of the energies of electronic excited states and the resulting X-ray spectra for benchmark systems through the development of a new, real-time coupled-cluster (CC) cumulant Green’s function approach.

Significance and Impact

The inclusion of double excitations and a correlated reference resulted in accurate core ionization potentials and reproduced satellite structures observed in X-ray photoelectron spectra measured at U.S. Department of Energy light sources.

Research Details

- We created a non-perturbative, time-evolution approach for calculating electronic correlations and excited states in molecules with a parallel implementation of time-dependent CC formalism.
- This approach naturally built nonlinear terms into the cumulant that are crucial for accurate quasi-particle and satellite properties.


Work was performed at University of Washington and Pacific Northwest National Laboratory.