Type: New
Title: "PRECISE: Predictive Electronic Structure Modeling of Heavy Elements"

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Scientific Discipline: Chemistry: Physical

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (400,000 Summit node-hours)

Research Summary: In this project, an international team will study frontier aspects of the physics and chemistry of molecules containing one or more heavy elements. The accurate treatment of molecular energies and properties of these elements requires inclusion of both relativistic and electron correlation effects. This has only recently become feasible due to the team's realization of a relativistic coupled cluster implementation that has been designed specifically for massively parallel GPU-accelerated supercomputers as part of the OLCF's Center for Accelerated Application Readiness program for Summit.

These applications will aid in the search for new physics beyond the Standard Model, unravel the complicated chemistry and spectroscopy of f-elements, and provide predictions for the chemical properties of superheavy elements. The project aims to set a new standard for accurate modelling of heavy elements and fill a large gap in the set of computational benchmark data for molecular systems. Filling this gap is for instance essential in the development of density functionals that can specifically target heavy elements. The project will thereby have an impact on computational chemistry that goes far beyond the results of the individual studies.