



Type: New

Title: "Predictive Electronic Structure Modeling of Heavy Elements"

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Scientific Discipline: Chemistry

INCITE Allocation:

Site: Oak Ridge National Laboratory

Machine (Allocation): IBM AC922 (490,000 Summit node-hours)

Research Summary: The PRECISE project will use highly accurate relativistic correlated electronic structure methods, implemented in a modern massively parallel gpu-accelerated code, to investigate different aspects of the chemistry and physics of transition metals and actinides, from their reactivity and spectroscopic signatures to their use as probes for physics beyond the Standard Model.

Accurate treatment of molecular energies and properties of these elements requires inclusion of both relativistic and electron correlation effects and 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 CAAR program for Summit and employed for the first time in the team's 2020 INCITE application.