

The EXtreme-scale Electronic Structure System (EXESS) and its applications

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Electronic structure theory calculations have the potential to predict matter transformations of strategic technological importance in drug discovery, synthetic biology, chemistry, and materials science that are currently too expensive or impossible to be characterized experimentally.

The main computational obstacle is that a predictive physicochemical characterization of these processes requires a large number of accurate electronic structure calculations on molecular system including multiple components and from hundreds to thousands of atoms.

Due to the computationally demanding nature of electronic structure calculations and to the complexity of modern high-performance computing hardware, quantum chemistry has so far failed to enable a matter transformation oracle that can operate at large molecular scales with an accuracy and speed that are useful in practice.

In this Lecture, I will discuss the making of an EXtreme-scale Electronic Structure System (EXESS) through the development of high-performance quantum chemistry algorithms that can fully take advantage of exascale-generation hardware including thousands of Graphics Processing Units (GPU) to perform accurate quantum chemistry calculations at unprecedented speed and molecular scales. I will complete the Lecture by showcasing how EXESS is enabling researchers to successfully tackle some of the grand challenges of our time in chemistry and material science.