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**From Petascale to Exascale: Prospects for Transforming Atomic, Molecular, and Chemical Dynamics
with Leadership Computing¹**
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Modeling and simulation with petascale computing has supercharged the process of innovation and understanding, dramatically accelerating time-to-insight and time-to-discovery. From petascale modeling of combustion for advanced engines, to designing bio-inspired catalysts for renewable energy, to exploring the evolution of complex systems such as our earth's climate, or breakthroughs gained from quantum many-body applications in chemical and nuclear physics, petascale computing is delivering high impact results that are transforming science and engineering. This presentation will provide an overview of the unique computational resources and user programs at the Oak Ridge Leadership Computing Facility (OLCF) at DOE's Oak Ridge National Laboratory, discuss a range of ambitious computational research projects underway in atomic, molecular, and chemical physics, and discuss scientific opportunities and challenges associated with advancing computational capabilities to the exascale.

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