AMES LABORATORY'S THEORY AND COMPUTATIONAL SCIENCES

Ames Laboratory
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Got GAMESS? Computational materials discovery, design, and characterization relies on advanced theories, innovative algorithms and associated software that predict material and chemical properties. All are areas in which Ames Laboratory excels.

Quantum chemistry: General Atomic and Molecular Electronic Structure System (GAMESS) is a leading ab initio quantum chemistry package, with over 250,000 downloads. Its large-scale use and computational linear-scaling make it an invaluable research and key acceptance code.

Electronic structure, atomistic simulations and dynamics: We develop innovative predictive methods for electronic, magnetic, structural, and dynamic properties in correlated-electron and non-equilibrium systems (e.g., Gützwiller methods for 4f and 5f electron magnets), large-scale atomistic simulation in complex materials, and spin dynamic techniques.

Finding NEMO: Ames Laboratory created global search optimization via genetic algorithms for crystal structure and grain boundary prediction of competing N-structural Energy-Minimum Objects (NEMO).

Transformation pathways and processing simulations: In concert with our experts in synthesis and crystal growth, we develop accurate methods to address competing phases and transition states as a guide to processing.

Complex alloy discovery and design: We develop predictive, multiple-scattering-theory-based electronic-structure methods to handle defects, disorder and thermodynamics that dictate most "real material" behavior, many of which drive technological use (e.g., alloyed magnets).

Complex, integrated systems: We build algorithms, heuristics and tools to model the complexity of our engineered, human, and natural systems, then develop integrated computational environments to enable informed, holistic decision making and design for these systems.

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U.S. DEPARTMENT OF ENERGY