

CSDM-A Program

In broad terms, the CSDM-A Program encompasses **experimental physical chemistry** and **applied computation**.

Systems span range of complexities...

- Isolated molecules and clusters
- Solutions
- Surfaces/interfaces
- Condensed phases
- Biological structures and systems.
- Molecular assemblies and nanomaterials

Of interest are projects that...

- Use and/or advance sophisticated experimental and/or modeling techniques that challenge how we think about fundamental physical phenomena.
- Computational projects typically have strong synergy with experiment.
- Provide fundamental insight into physical phenomena underpinning emerging technologies in areas of national importance, and NSF priorities.

CTMC Program

The Chemical Theory, Models, and Computational Methods (CTMC) supports the development of new theoretical methods/models to address chemical challenges.

Topic areas include...

- Electronic structure theory
- Biosimulation
- AI / Machine Learning
- Molecular Dynamics / Statistical Mechanics
- Quantum Dynamics / Spectroscopy

Of interest are projects that...

- Develop theoretical methods or modeling techniques that challenge how we think about fundamental physical phenomena.
- Enable prediction and interpretation of experiments.
- Provide the tools to gain fundamental insight into physical phenomena underpinning emerging technologies in areas of national importance, and NSF priorities.

NSF Priority Areas

- **Quantum Information Science (QIS):** Exploitation of quantum phenomena (e.g., coherence, superposition, entanglement and squeezing) for next generation technologies in sensing, computing, and communication.
- **Critical Aspects of Sustainability (CAS):** Advancement of innovative solutions to climate change and clean energy problems, as well as sustainable technologies that improve efficiency of natural resource utilization.
- **Artificial Intelligence (AI):** Development and application of AI-inspired techniques (e.g., machine learning and deep learning) in modeling and simulation, data and model analytics, concept discovery, and physical systems/experiment.
- **Computational and Data-Enabled Science and Engineering (CDS&E):** Utilization of large-scale computation and large-scale data to advance knowledge and accelerate discovery.