

## The Molecular Sciences Software Institute

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**Abstract:** The Molecular Sciences Software Institute (MolSSI) is a nexus for science, education, and cooperation serving the worldwide community of computational molecular scientists — a broad field including of biomolecular simulation, quantum chemistry, and materials science. The Institute, which was recently funded by the National Science Foundation as part of the White House’s National Strategic Computing Initiative, will spur significant advances in software infrastructure, education, standards, and best-practices that are needed to enable the molecular science community to open new windows on the next generation of scientific Grand Challenges, ranging from the simulation of intrinsically disordered proteins associated with a range of diseases to the design of new catalysts vital to the global chemical industry and climate change. The MolSSI will enable the computational molecular science community to work together to leverage its diverse capabilities that will reduce or eliminate the gulf that currently delays by years the practical realization of theoretical innovations. Ultimately, the Institute will enable computational scientists to tackle problems that are orders of magnitude larger and more complex than those currently within our grasp. This lecture will provide an overview of the Institute’s structure, goals, and vision.