York Lab
https://theory.rutgers.edu

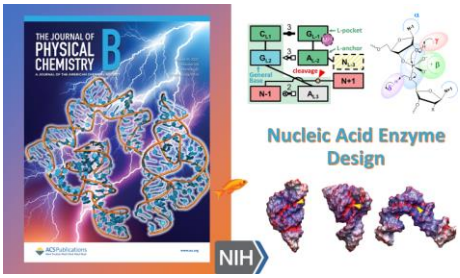
RUTGERS THE STATE UNIVERSITY OF NEW JERSEY
IQB
Laboratory for Biomolecular Simulation Research

York Lab – Recruiting Graduate Students: https://Theory.Rutgers.edu

The York Lab at Rutgers is at the forefront of technology development for advanced molecular simulations, and co-develops the **Amber** software package. We design new highly accurate force fields that integrate quantum chemistry with artificial intelligence and can be applied with novel enhanced sampling and free energy methods to provide predictive insight into a wide range of problems. Of particular interest is the study of reaction paths and catalytic mechanisms central to nucleic acid enzyme design, and molecular recognition and binding events important for drug discovery. **Research areas are:**

Drug Discovery

Alchemical free energy (AFE) simulations are a vital part of computer-aided drug discovery, and are used to predict the binding affinities of proposed drug-like molecules to their protein or RNA targets. The York Lab develops the state-of-the-art AFE methods in the Amber software package that boasts one of the fastest GPU-accelerated free energy simulation engines and is used by pharmaceutical companies worldwide. Our FE-ToolKit software provides powerful network-wide analysis of ligand data sets with integration of theoretical and experimental constraints. The methods are interoperable with our Deep-learning potentials (such as "QDπ") for high accuracy.

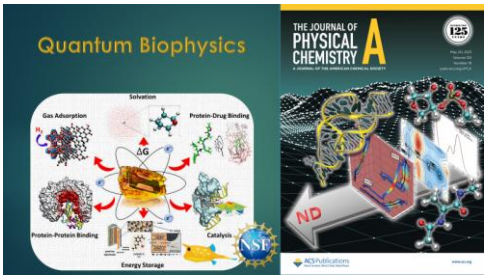


Nucleic Acid Enzyme Design

The York Lab brings to bear state-of-the-art theoretical methods and new machine-learning models to the study of the catalytic mechanisms of naturally occurring RNA enzymes (or "ribozymes") as well as artificially engineered RNA and DNA enzymes, and new enzymes built from synthetic nucleic acids that form artificially expanded genetic information systems. A goal of this work is to characterize the diverse array of catalytic strategies available to these molecules in order to elucidate guiding principles for nucleic acid enzyme design that may lead to new biotechnology and therapeutics.

Deep-Learning Potentials

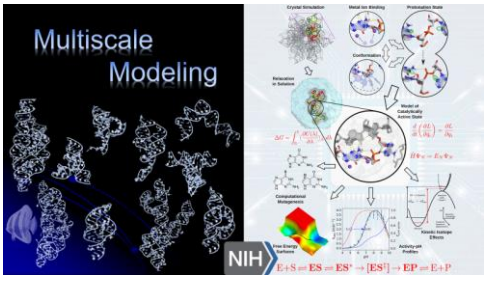
Artificial intelligence and deep-learning methods are revolutionizing science, and nowhere are these breakthroughs more exciting than in computational chemistry. The York Lab uses AI methods to facilitate molecular dynamics simulations by developing new deep-learning potentials that offer the accuracy of *ab initio* quantum chemical methods (and beyond!) for affordable computational cost. These potentials enable applications to studies of enzyme catalysis and ligand-protein binding free energy prediction with unprecedented accuracy.



Quantum Biophysics

Biological systems present special challenges for the application of quantum chemical models. In to treat very large systems, quantum methods based on density-functional theory must be formulated to be highly efficient and to scale linearly with system size. The York Lab develops novel AI-enhanced quantum mechanical force fields that are able to be applied in large-scale simulations. These methods enable problems of biomolecular reactivity and drug-target interactions to be computed with very high accuracy at low computational cost, widening the scope of applications that can be addressed.

Multiscale Modeling



Multiscale modeling involves the integration of a hierarchy of theoretical methods that work in concert to address complex chemical problems that span a wide range of spatial and temporal scales. The York Lab develops a number of multiscale modeling tools including: combined quantum mechanical/molecular mechanical+machine-learning potentials (QM/MM-ΔMLPs), fast linear-scaling electrostatic methods (generalized fast-multipole and PME/Ewald), methods for accurate computation of free energy surfaces and pathways in high dimensions, and new methods for enhanced sampling. These tools are used to make experimentally testable predictions and guide the design of new technology.

Join Us!

The **York Lab** is actively recruiting talented scientists to join our team. If you are a prospective graduate student, check out our Research and apply now to our graduate program in Chemistry & Chemical Biology or Quantitative Biomedicine, or contact us about opportunities!