Theoretical Chemistry and Chemical Physics

Iyengar Group

We develop new theoretical methods and implement these into efficient computational algorithms to solve problems in biophysical chemistry, atmospheric chemistry, and nanomaterial science. Our research lies on the interface of chemistry, computational physics, and applied mathematics.

Principal areas of study:
- Development of new computational methods for dynamical treatment of nuclei and electrons
- Study of hydrogen transfer reactions in biological enzymes
- Non-equilibrium electron transport in donor-bridge-acceptor systems
- Vibrational analysis and energy redistribution in hydrogen bonded and atmospheric systems

The descriptions below are hyperlinked.

Quantum Dynamics of electrons and nuclei
We develop new methods for simultaneous quantum mechanical treatment of electrons and nuclei. These methods involve approximate treatments that facilitate the study of large complex phenomena in biological and atmospheric processes.

Electron transport in open, non-equilibrium systems:
Electron transport through donor-bridge-acceptor systems plays an important role in many materials and biological problems. Specifically, in molecular electronics, the interface coupling between the electron donor molecules and bridge molecule, convert the system into an open non-equilibrium problem. We develop new approaches to treat these problems. Critical hallmarks of the methods we have developed (a) these include the rigorous treatment of open system boundary conditions using offsetting absorbing and emitting boundary conditions, (b) nuclear and non-equilibrium electronic dynamics is constructed in the presence of external fields.

Simulating complex biological phenomena:
Hydrogen transfer reactions are significant in many biological and atmospheric processes. Due to its light mass, the hydrogen transfer reactions show propensity to demonstrate unexpected quantum effects arising from the nuclei. These are experimentally noted through unexpected isotope effects. We develop rigorous computational methods that include quantum effects arising from electrons and nuclei to treat these complex problems.

Vibrational Analysis of hydrogen bonded clusters and atmospheric systems:
Fundamental studies on hydrogen bonded clusters and atmospheric reactions allow deduction of energy redistribution pathways and associated temperature dependences. These (a) demonstrate connections between different experimental techniques, and (b) provide atmospheric reactions rates including non-statistical behavior. The computational approaches involve a time-dependent spectroscopic analysis, constructed from dynamical treatment of electrons and nuclei.

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