DEPARTMENT OF CHEMISTRY

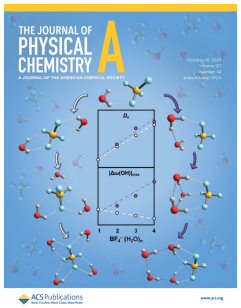
MISSOURI UNIVERSITY OF SCIENCE AND TECHNOLOGY

Computational Quantum Chemistry: Theory and Applications

Accelerating Discovery with Theory, Computation, Modeling and Simulation

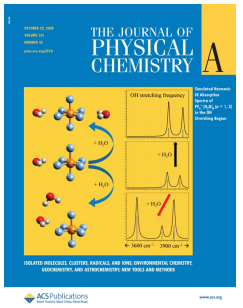
- Prediction of molecular structure and properties with computational quantum chemistry
- Development of new theoretical/computational methods for non-covalent clusters
- Water clusters and explicit hydration/solvation
- Vibrational and rotational spectroscopy
- Intermolecular and intramolecular non-covalent interactions (hydrogen bonding, halogen bonding, π-stacking, etc.)
- Proton transfer and hydrogen atom transfer processes
- Quantifying aromaticity through nucleus independent chemical shifts (NICS) analyses
- Guiding conformational/structural exploration of chemical space with machine learning / artificial intelligence
- Computationally informed design of organic chromophores and building-blocks for optoelectronic devices/materials

Energetics and Spectroscopic Signatures of Ion Hydration

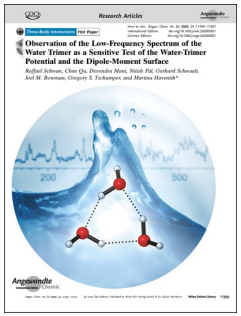


Featured on two recent covers of *J. Phys. Chem. A*

Vol 124, pp 8744-8752 (2020)
DOI:10.1021/acs.jpca.0c06466
Vol 127, pp 8806-8820 (2023)
DOI: 10.1021/acs.jpca.3c04014



Good Experiment + Good Theory = Great Science



Probing cooperative effects in hydrogen bonding
Frontispiece feature in *Angew. Chem. Int. Ed.*

Vol 59, pp 11399-11407 (2020)
DOI: 10.1002/anie.202003851

News releases from NSF and ScienceDaily

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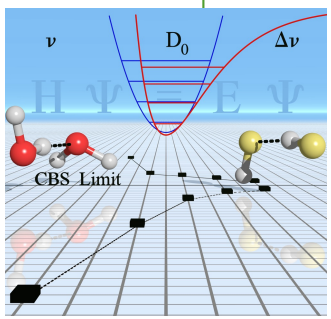

Keywords

Physical chemistry; computational chemistry; quantum chemistry; non-covalent interactions; hydrogen bonding; halogen bonding;

Significant Achievements and Recognitions

- 14 journal covers/artwork featuring research
- >125 peer-reviewed articles
- h-index: 40; citations: >5,800
- AAAS Fellow

Updated Sept. 2024

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https://sites.mst.edu/quantumchem