

QMC Electronic Structure

Objective: Develop Quantum Monte Carlo (QMC) methods to stochastically solve many-body electronic structure problems.

Implications: Accurately predict or explain chemical phenomena where other methods fail or aren't applicable.

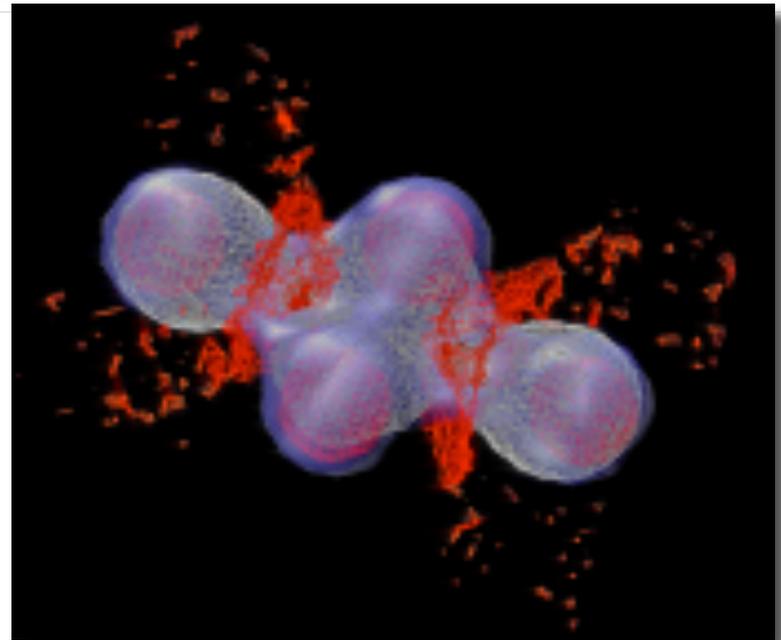
Accomplishments: Developed hybrid QMC / Molecular Mechanics formalism.

- Obtained interaction energy of a 2-water cluster treating one H₂O quantum mechanically and other classically; prelude to effort to find much sought-after electron binding energy in (H₂O)_n.
- Studied series of Li clusters in different charge states to obtain energies for cluster growth, charge, and discharge in interactions with graphene.

NERSC:

- ZORI scales to 32k cores on Franklin

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Cluster of four Li atoms and electron cloud (red) as calculated by ZORI on NERSC's Cray XT4