Describing Chemical Dynamics with Quantum Simulators

Quantum simulations with trapped ions

• Simulating molecules with numerical methods are only applicable to small molecules in a limited parameter regime.
• Trapped-ion systems are a promising platform for quantum computation and quantum simulations.
• We have used trapped-ion systems to study charge flow in molecules.

Quantum simulations

• We have compared the performance of trapped-ion quantum simulations with two classical algorithms, tDMRG and Ehrenfest, by simulating the dynamics of a toy model system.
• Quantum simulators reduce the required simulation time.

Mapping molecules to trapped ions

• Molecules are commonly described by mathematical expressions known as Hamiltonians.
• The molecular Hamiltonians can be mapped to trapped-ion Hamiltonians to perform exact simulations of chemical processes.

Chemical problems to study

Conical intersections
Vibrationally-assisted ET
Polarized light ET
CISS effect