

Mixed Quantum/Classical Dynamics with Full CI:

Correlation and Exchange in Condensed Phases

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We have developed a new method for performing mixed QM/CM simulations using full configuration interaction (CI), including spin.⁽¹⁾

Using the method, we have calculated the structure and dynamics of hydrated dielectrons (two excess electrons in a single cavity in liquid water), with charge densities and solvent structures of singlet and triplet states shown at right.⁽²⁾ It is clear that exchange, spin and correlation affect both the structure and dynamics of the classical solvent molecules.

Studies in progress using our method include:

Photodetachment from many- e^- atoms

Spin flips and decoherence--loss of entanglement

Time-resolved spectroscopy in condensed phases

(1) Larsen and Schwartz, J. Chem. Phys. **119**, 7672 (2003).

(2) Larsen and Schwartz, J. Phys. Chem. B **108**, 11760 (2004).

