Induction in Chemistry: Introducing Electrostatic Bonds

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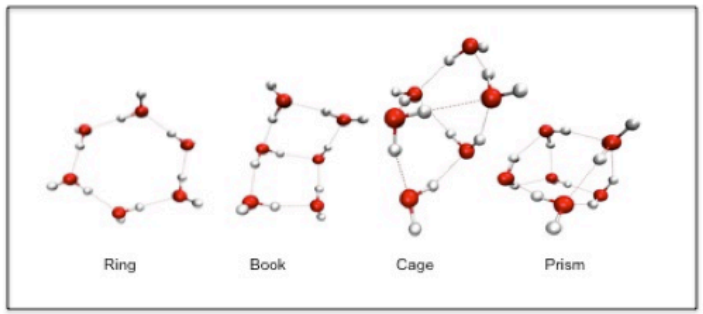
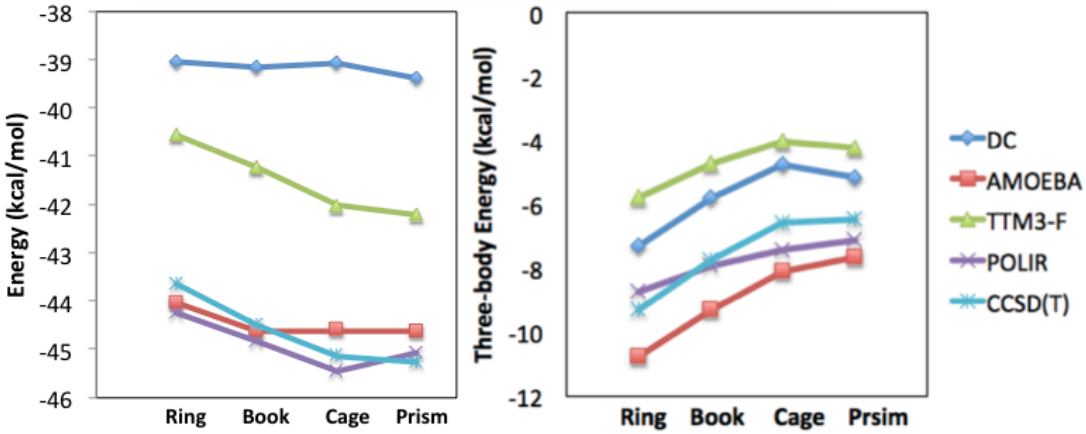
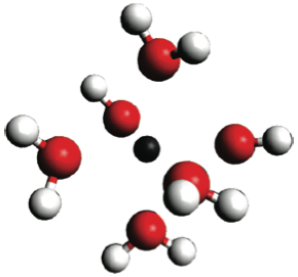
With a careful treatment of polarization at short range, classical methods describe a surprising number of phenomena generally considered to require quantum mechanics.

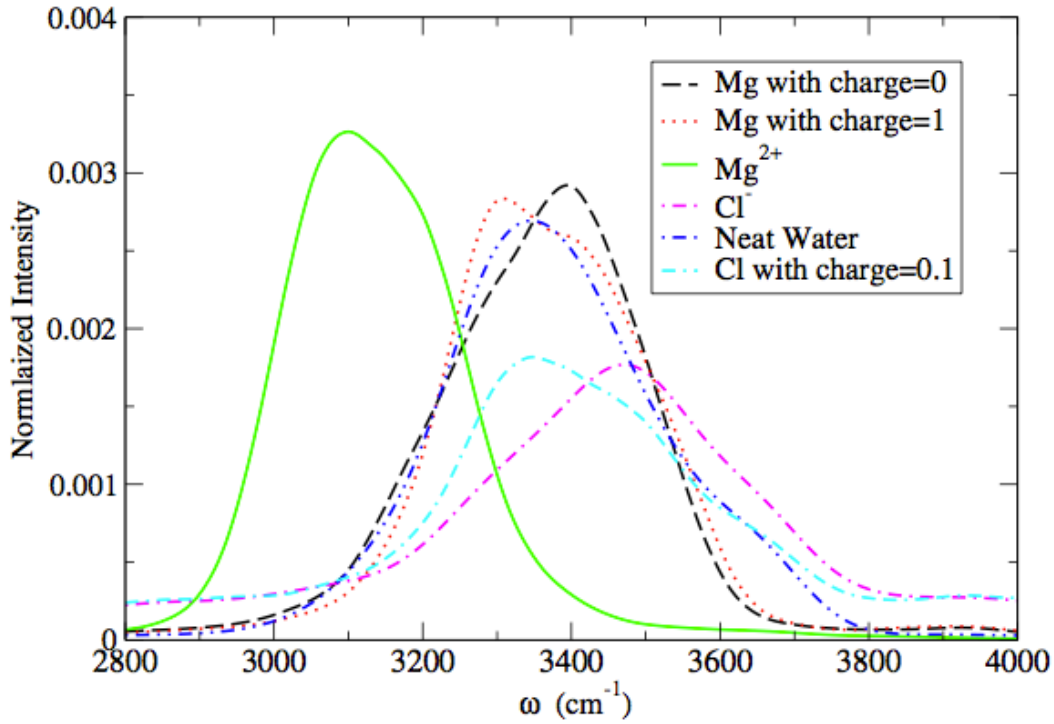
Classical cluster energies of the POLIR water potential approach high-level quantal results (CCSD(T)) for $(H_2O)_6$, and are superior to those from existing polarizable potentials.





The energy and structure of hexa-coordinated Cu^{2+} are described by classical electrostatic bonds





IR solution spectra from the classical dipole correlation: Mg^{2+} has a large redshift and Ca^{2+} is broad and weakly blueshifted, in agreement with experiment. “Synthetic” solutes correctly obey: Mg^{+1}, hydrophilic, red- and blueshifted shoulders; Mg^{0}, weakly hydrophilic, slight blueshift; $Cl^{+0.1}$, hydrophobic, slight redshift.