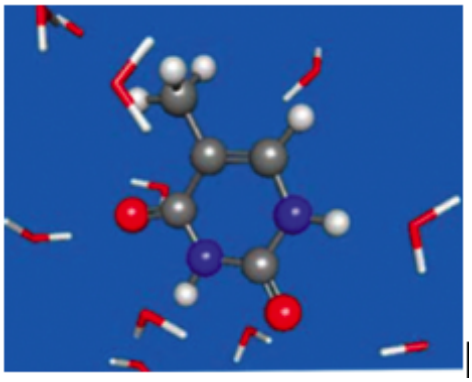
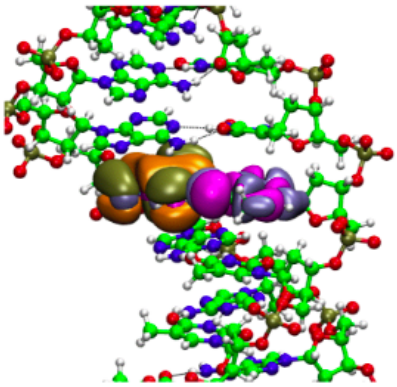
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Treating Environmental Effects: Implicit and Explicit Solvent Models

- **Popular implicit solvation models:**
  - SM8, SM12, SMD, COSMO, C-PCM, SS(V)PE, IEF-PCM, CMIRS, and more;
  - Intrinsically smooth discretization of the solute/continuum interface;
  - Poisson equation solver for anisotropic dielectric boundary conditions.
- **Effective fragment potential (EFP) for modeling explicit solvent with polarizable embedding:**
  - Available for ground and excited states;
  - Interfaced with DFT and wave function based methods;
  - Extension to biomolecules is available;
  - Built-in library of effective fragments.
- **Density embedding is available for selected methods.**
- **Many-body expansion can incorporate solvent molecules at a QM level.**
- **Stand-alone electrostatic embedding (QM/MM) capabilities:**
  - Available for ground or excited states;
  - Integration with PCM models (QC/MM/PCM);
  - Many-body expansion can incorporate solvent molecules at a QM level.
- **Interface to CHARMM:**
  - QM/MM using CHARMM's extensive set of sampling methods;
  - Full QM/MM Hessian or "mobile block-Hessian" approximation facilitate study of vibrational entropic effects or large-scale conformational changes.
- **Interfaces with GROMACS and NAMD are available.**



(a) EFP used to compute ionization energies and redox potentials of bulk-solvated species



(b) HOMO and LUMO of a Watson-Crick base pair in a QM/MM description of double-stranded DNA

Request a free trial at www.q-chem.com