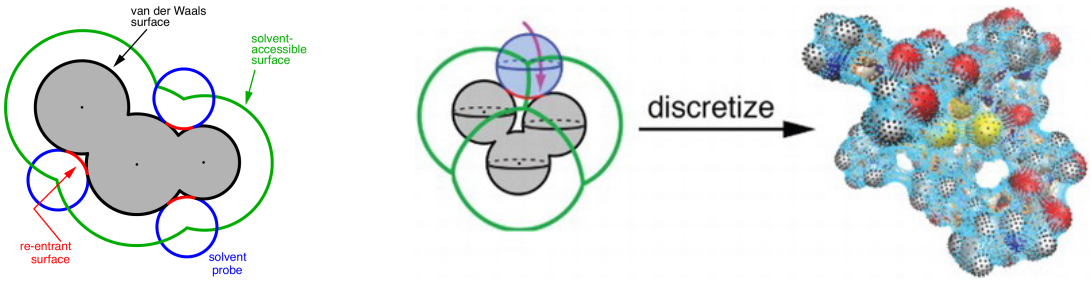
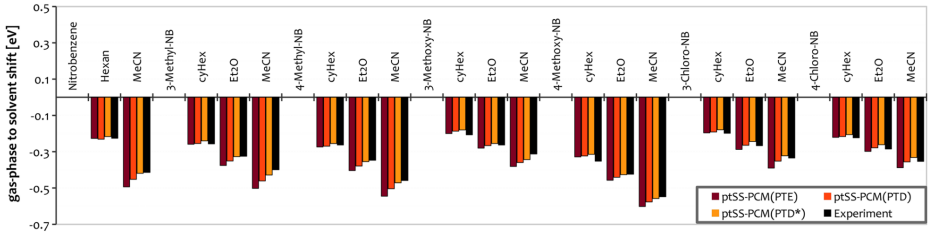
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Dielectric Continuum Solvation Models



In implicit solvation models the solvent is coarse-grained as a dielectric continuum, of which the electrostatics is described by Poisson or Poisson-Boltzmann equation. In polarizable continuum models (PCMs) apparent surface charge is treated by self-consistent reaction field models, reducing a 3D volumetric polarization problem into a 2D surface charge problem. Q-Chem features:

- C-PCM, COSMO, SS(V)PE/IEF-PCM;
- Implementation employs a Switching/Gaussian (SWIG) discretization scheme, which resolves the long-standing potential energy surface discontinuity issue;
- An iterative conjugate gradient (CG) solver is used to solve the surface charge equation to achieve linear scaling;
- Isodensity SS(V)PE eliminates the empiricism associated with cavity construction;
- Solvation energy beyond electrostatic interaction: nonelectrostatic models including SM8, SM12, SMD and CMIRS;
- Nonequilibrium solvation effect in excitation, ionization and emission: linear-response (LR) and state-specific approaches;
- PCM is supported in post-HF theories: MP2, ADC and CC/EOM-CC, and also in energy decomposition analysis (ALMO-EDA).



Experimental and calculated solvent shifts at the ADC(2)/ptSS-PCM level of theory with the PTE, PTD, and scaled PTD* approaches

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