We have developed a new charge-density based solvation model called SMD. The SMD algorithm involves an integration of the nonhomogeneous Poisson equation for electrostatics. The SMD model has been parametrized using a large training set of neutral and ionic solvation free energies for various solutes in water and organic solvents (nearly 3000 data). The non-bulk-electrostatic part of the SMD model utilizes the cavity–dispersion–solvent-structure formalism that was worked out for previous solvation models developed at the University of Minnesota.

The figures demonstrate the significant improvement in the quality of IEFPCM/Gaussian 03, CPCM/GAMESS, and GCOSMO/NWChem upon using the SMD parameters instead of the default settings for the current implementations of these models in Gaussian 03 (G03), GAMESS, and NWChem (note: MUE stands for mean unsigned error, that is, mean absolute deviation from a set of accurate data).
M06 functionals are the most accurate density functionals with broad applicability in chemistry. The development of these functionals and their application to complex projects in supramolecular and zeolite chemistry was promoted by the ability to run large calculations as part of the Grand Challenge project.