1086-92-1937 **J. Che*** (jche@gnf.org), **Z. Guo** (zguo@gnf.org), **B. Li** (bli@math.ucsd.edu), **L. Cheng** (lcheng@math.ucsd.edu) and **J. Dzubiella** (jdzubiel@physik.hu-berlin.de). *Hydration Free Energy from a Variational Implicit Solvent Model.*

Hydration free energy is an important properties for organic and bio molecules involved in drug discovery industry. Explicit water simulations are usually too time consuming for daily industrial applications, and conventional implicit solvent models lack the self-consistency between polar and non-polar interactions. Recently, we developed a variational implicit solvent model (VISM) that treats polar and non-polar interactions self-consistently. Here, we applied it to a large set of diverse small organic molecules as well as protein complexes, and demonstrate its capability to accurately reproduce the hydration free energy with far fewer adjustable parameters. In addition to providing more accurate physical insights into the solvation process, the efficiency of the numerical implementation through level set equations allows the calculations to be of practical use in industrial settings. (Received September 24, 2012)