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Atomistic Models for High-throughput Prediction of Hydration Free Energies JIANZHONG WU, University of California, Riverside, CA 92521 — The classical density functional theory (DFT) is proposed as an efficient computational tool for high-throughput prediction of the solvation free energies of small molecules in liquid water at the ambient condition. With the solute molecules represented by the AMBER force field and the TIP3P model for the solvent, the new theoretical method predicts the hydration free energies of 500 neutral molecules with average unsigned errors of 0.96 kcal/mol and 1.04 kcal/mol in comparison with the experimental and simulation data, respectively. The DFT predictions are orders of magnitude faster than conventional molecular dynamics simulations and the theoretical performance can be further improved by taking into account the molecular flexibility of large solutes.

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