Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Solvation dynamics and enzyme catalysis in a designed enzyme undergoing directed evolution CARL SCHRECK, Lawrence Berkeley National Laboratory, TERESA HEAD-GORDON, University of California, Berkeley — We explore whether catalysis of a de novo designed enzyme-substrate complex is correlated to necessary solvent fluctuations to induce a chemical reaction. By studying a designed KEMP Eliminase as it goes through rounds of directed evolution to improve it's catalytic activity, we have found that catalytic activity correlates with an increase in density and structure of water near the active site. This suggests fluctuations in the solvation water near the active site couple to fluctuations in KEMP Eliminase to facilitate the catalytic process. To flesh this idea out, we are studying the progression of vibrational properties and cooperative fluctuations of solvation water by simulating the terahertz observable.

Carl Schreck
Lawrence Berkeley National Laboratory

Date submitted: 15 Nov 2013 Electronic form version 1.4