Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Solvated dissipative electro-elastic network model of hydrated proteins DANIEL MARTIN, Arizona State University — Elastic network models coarse grain proteins into a network of residue beads connected by springs. We add dissipative dynamics to this mechanical system by applying overdamped Langevin equations of motion to normal-mode vibrations of the network. In addition, the network is made heterogeneous and softened at the protein surface by accounting for hydration of the ionized residues. Solvation changes the network Hessian in two ways. Diagonal solvation terms soften the spring constants and off-diagonal dipole-dipole terms correlate displacements of the ionized residues. The model is used to formulate the response functions of the electrostatic potential and electric field appearing in theories of redox reactions and spectroscopy. We also formulate the dielectric response of the protein and find that solvation of the surface ionized residues leads to a slow relaxation peak in the dielectric loss spectrum, about two orders of magnitude slower than the main peak of protein relaxation. Finally, the solvated network is used to formulate the allosteric response of the protein to ion binding. The global thermodynamics of ion binding is not strongly affected by the network solvation, but it dramatically enhances conformational changes in response to placing a charge at the a the active site.

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Date submitted: 09 Nov 2012 Electronic form version 1.4