Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

**Machine learning of single molecule free energy surfaces and the impact of chemistry and environment upon structure and dynamics** RACHAEL MANSBACH, ANDREW FERGUSON, Univ of Illinois - Urbana — The conformational states explored by proteins and polymers can be controlled by environmental conditions (e.g., temperature, pressure, solvent) or molecular chemistry (e.g., chain length, side chains). It is of fundamental interest to quantify the impact upon molecular structure and function, and a prerequisite to the rational engineering of proteins and polymers with desired properties. Using the diffusion map nonlinear manifold learning algorithm, we have developed an approach to: (i) extract from molecular simulations the single molecule free energy surface governing the microscopic molecular behavior, (ii) quantify changes in its topography as a function of environmental conditions and molecular chemistry, and (iii) relate these perturbations to changes in molecular structure and dynamics. In a first application to an $n$-eicosane chain, we have quantified the thermally accessible chain configurations as a function of temperature and solvent conditions. In a second application to a family of polyglutamate-derivative decameric homopeptides, we quantify the stability of the helical state relative to the random coil as a function of side chain length and expose the molecular mechanism underpinning side chain-mediated helix stability.

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Date submitted: 24 Oct 2014 Electronic form version 1.4