Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

AP helical stability in salt solutions ELIANA ASCIUTTO, Duquesne University, KAN XIONG, University of Pittsburgh, SANFORD ASHER, University of Pittburgh, JEFFRY MADURA, Duquesne University — Protein dynamics depends on the environment and the inclusion of salts in the simulation of folding/unfolding becomes extremely necessary when comparing energy barriers or reaction rates with experimental results. The aim of this study is to investigate the effects of three sodium salts: $NaClO_4$,$NaCl$ and Na_2SO_4 on the helical stability of AP, a mainly alanine peptide. The dependence of the peptide helical stability on the environment has been studied using Replica Exchange Molecular Dynamics (REMD) simulations, Circular Dichroism (CD) and Ultraviolet Raman Resonance Spectroscopy (UVRS) experiments. It was found that $NaClO_4$ solution strongly stabilizes the helical states and that the order in which sodium salts stabilize the peptide helical states follows a reverse Hofmeister Series ($ClO_4^- < Cl^- < SO_4^{2-}$). Another interesting result found is that ClO_4^- ions are attracted to the backbone; Cl^- ions are repelled while SO_4^{2-} ions are attracted to the positive side chains. A thorough investigation of the ion effects on the first and second solvation water along with the Kirkwood-Buff theory for solutions allowed us to explain the physical mechanisms involved in the observed ion specific effects.

Eliana K. Asciutto
Duquesne University

Date submitted: 25 Nov 2008 Electronic form version 1.4