Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Roles of urea and TMAO on the interaction between extended non-polar peptides ZHAOQIAN SU[1], CRISTIANO DIAS[2], New Jersey Inst of Tech — Urea and trimethylamine n-oxide (TMAO) are small molecules known to destabilize and stabilize, respectively, the structure of proteins when added to aqueous solution. To unravel the molecular mechanisms of these cosolvents on protein structure we perform explicit all-atom molecular dynamics simulations of extended poly-alanine and polyleucine dimers. We use an umbrella sampling protocol to compute the potential of mean force (PMF) of dimers at different concentrations of urea and TMAO. We find that the large non-polar side chain of leucine is affected by urea whereas backbone atoms and alanine's side chain are not. Urea is found to occupy positions between leucine's side chains that are not accessible to water. This accounts for extra Lennard-Jones bonds between urea and side chains that favors the unfolded state. These bonds compete with urea-solvent interactions that favor the folded state. The sum of these two energetic terms provide the enthalpic driving force for unfolding. We show here that this enthalpy correlate with the potential of mean force of poly-leucine dimers. Moreover, the framework developed here is general and may be used to provide insights into effects of other small molecules on protein interactions. The effect of the TMAO will be in the presentation.

[1]Department of Physics, University Heights, Newark, New Jersey, 07102-1982
[2]Department of Physics, University Heights, Newark, New Jersey, 07102-1982

Zhaoqian su
New Jersey Inst of Tech

Date submitted: 06 Nov 2015 Electronic form version 1.4