Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Behavior of aqueous solutions in hydrophobic confinement studied using molecular simulations SUMIT SHARMA, Ohio University — Biological processes, such as formation of cell membranes, vesicles and folding of protein molecules, entail formation of a predominantly hydrophobic interior devoid of water. These processes occur in crowded aqueous environments comprising of amino acids, carbohydrates, ionic species, protein molecules, etc. Kinetics of these processes involve drying of hydrophobic pockets. Previous studies reveal that the kinetics of evaporation of water in hydrophobic confinement significantly slow down as the confinement gap increases. Presumably, the constituents of aqueous environment in biological systems modulate the kinetics of evaporation of confined water. In this work, we employ forward flux sampling in molecular dynamics simulations to study the role of solutes at different concentrations in modulating the kinetics and mechanism of evaporation of water under hydrophobic confinement. The results of these simulations will be useful for understanding optimum conditions for protein folding and other biological self-assembly processes.

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Date submitted: 05 Nov 2015 Electronic form version 1.4