Abstract Submitted
for the SES16 Meeting of
The American Physical Society

Evaporation of Water in Hydrophobic Confinement MOHSEN GHASEMI, Department of Mechanical Engineering, Ohio University, Athens, OH 45701, SUMIT SHARMA, Department of Chemical and Biomedical Engineering, Ohio University, Athens, OH 45701, OU SIMULATION TEAM — Evaporation of water from hydrophobic pockets has been thought to play an important role in many biomolecular assembly processes such as folding of globular proteins, formation of cell membranes, aggregation of fibrils etc. Hence, understanding the thermodynamics and kinetics of this phenomenon is important for delineating the underlying mechanisms of these processes. Since liquid to vapor transition of water under hydrophobic confinement is an activated event, Indirect Umbrella Sampling (INDUS) method has been applied in molecular dynamics simulation to determine the magnitude of the free energy barrier associated with the transition under varying conditions.

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Date submitted: 04 Oct 2016 Electronic form version 1.4