Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Molecular Modeling of a Probe in 2D IR Spectroscopy ANTHONY COOPER, LUCA LARINI, Rutgers University-Camden — Proteins must adopt a precise three dimensional structure in the folding process in order to perform its designated function. Although much has been learned about folding, there are still many details in structural dynamics that are difficult to characterize by existing experimental techniques. In order to overcome these challenges, novel infrared and fluorescent spectroscopic techniques have recently been employed to probe the molecular structure at the atomistic scale. These techniques rely on the spectroscopic properties of the nitrile group attached to a phenylalanine. In this study, we model this probe and we compute its properties in different solvents. This is done by performing Molecular Dynamics simulations with a PheCN solvated in water, urea and TMAO. We measure the decay rate of the vibrational stretching of the CN group in order to characterize the effects of different solvents on the local structure of the molecule. This data can be used to identify non-trivial conformational changes of the protein in the folding process. Preliminary results show agreement with current experimental data on 2D IR spectroscopy.

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Date submitted: 13 Nov 2016 Electronic form version 1.4