Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Interactions of Lysozyme and Azobenzene Derivatives in the Solution and on a Surface TAO WEI, Lamar University, KATHERINE SHING, Mork Family Department of Chemical Engineering & Materials Science, Los Angeles, CA 90089-1211 — The reversible isomerization of the azobenzene and its derivatives can control protein structure in an aqueous environment with the alternation of visible and UV lights for very promising applications in drug delivery. However, an atomistic description of Azo-molecules and protein amino acid residues is still lacking. In this study we performed atomistic molecular dynamics simulation to study the interactions between a lysozyme molecule and the Azobenzene derivative (in the bulk solution and grafted on the Silica surfaces). Protein structural arrangements (i.e., the shape and secondary structures) and its mobility, as a function of tran/cis ratio in the bulk solution and on the self-assembling monolayer surface's density and morphology, are systematically investigated.

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Date submitted: 24 Nov 2014 Electronic form version 1.4