Abstract Submitted
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Molecular Dynamics Simulation of Alkanethiol Monolayer with Azobenzene Molecule on the Au(111) Surface[1] PING JIANG, ADRIAN ROITBERG, JEFFREY KRAUSE, Department of Chemistry, University of Florida, HAI-PING CHENG, Department of Physics, University of Florida — Azobenzene-based molecules have been investigated widely in various applications, such as optomechanical devices and switching elements for microelectronics. A heterogeneous system consisting of an alkanethoil (dodecanethiol) monolayer with azobenzene (trans and cis) molecules on a Au(111) surface has been studied using classical molecular dynamics (MD) to control and predict the properties of this system. The temperature dependence of the tilt angle and diffusion properties of the molecule on the surface have been analyzed in detail compared to the corresponding homogeneous system. Finally, we discuss the implications of our results for the interpretation of recent experiments.

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Ping Jiang
Department of Chemistry, University of Florida

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