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Atomic motion and electronic structure of alkanethiol monolayer covered gold surfaces[1] SABRI ALKIS, HAI-PING CHENG, JEFFREY KRAUSE, University of Florida — Self-assembled alkanethiol monolayers are subjects of great interest because of potential applications in future nano-electronics. In this talk, we report our recent studies of the motions of Au atoms on alkanethiol monolayers using molecular dynamics in conjunction with first-principles calculations. Guided by accurate quantum mechanical calculations, we have calibrated the interactions between Au atoms and monolayers for classical simulations. We then investigate the motions of Au atoms as a function of coverage and temperature. Simulations with improved potential parameters show a good agreement with experimental observations. In addition, we discuss the electronic structure and charge transfer at the interface between the molecular monolayer and gold (111) surfaces.

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