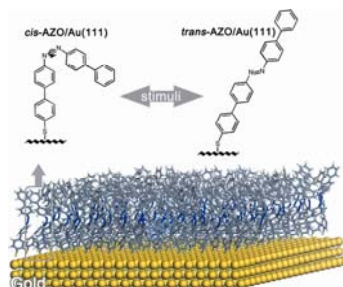


Reactive molecular dynamics simulations of switching processes of azobenzene-based monolayer on surface

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Theoretical simulation of the switching process of the self-assembled monolayer (SAM) on the metal surface is a challenge due to the complicated composition with thousands of atoms and triggering by the quantum-mechanical events. A molecular dynamics simulation with the reactive rotation potential of N=N bond^{1,2} is implemented to investigate the dynamic conformational changes and packing effects on the isomerization of the terminally thiol functionalized azobiphenyls (AZOs). To distinguish the time evolutions that start from *cis* and *trans* initial configurations, respectively, two different functions are established to model the potential energy curves of *cis*-to-*trans* and *trans*-to-*cis* transitions, instead of the only one cosine function used in the conventional non-reactive force fields. In order to simulate the conformation transitions of the AZO film on surface, a random switching function, dependent on the N=N twisting angle, is constructed to consider both forward and backward *cis/trans* isomerization events and to trigger the reaction by changing the N atom types automatically. Furthermore, three azobenzene derivate self-assembled monolayers are found not only tunable with changes in wave length of ultraviolet-visible light, but also with directions of electric filed on the Au(111) surface.



References

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