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Theoretical study of photoisomerization of azobenzene derivatives on Au(111)[1] DAVID A. STRUBBE, MATTHEW J. COMSTOCK, NIV LEVY, ARMEN KIRAKOSIAN, JONGWEON CHO, MICHAEL F. CROMMIE, STEVEN G. LOUIE, Department of Physics, University of California, Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory — Azobenzene and its various substituted derivatives are organic molecules that can be made to photoisomerize reversibly in solution between the *cis* and *trans* isomers. Scanning tunneling microscopy (STM) experiments have recently shown that photoisomerization is also possible in vacuum on a Au(111) surface. We use *ab initio* pseudopotential density-functional theory to confirm and analyze the experimental results by simulating STM images of the isomers, and we also study how the molecules adsorb on the surface and why some azobenzene derivatives can photoisomerize on the surface while others cannot.

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