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Selective Chemical Raman Enhancement for Organic Adsorbates at Metal Surfaces[1] ALEXEY T. ZAYAK, Molecular Foundry, LBNL, Berkeley, CA 94720, Department of Electrical Engineering and Computer Sciences, UC Berkeley, CA 94720, USA, YING HU, Bioengineering Department, Rice University, Houston, TX 77005, HYUCK CHOO, Molecular Foundry, LBNL, Berkeley, CA 94720, Department of Electrical Engineering and Computer Sciences, UC Berkeley, CA 94720, USA, STEFANO CABRINI, P. JAMES SCHUCK, JEFFREY B. NEATON, Molecular Foundry, LBNL, Berkeley, CA 94720 — It has long been observed that in surface enhanced Raman spectroscopy (SERS) relative mode intensities differ from gas- and solution-phase data, which obscures understanding of SERS in general. Using first-principles methods, we examine how chemisorption affects Raman scattering of molecules on metal surfaces relative to gas-phase, and provide a quantitative description of this effect. Calculated Raman spectra for benzene thiol bound at different sites on Au(111) show that chemical enhancement arises from the mode dependent electron-phonon coupling of the metal-molecule interface. Site-dependent enhancements are explained correlated to interfacial electronic structure. Comparison to experiments suggests affinity of benzene thiol for bridge sites on Au(111) surfaces.

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