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Vibrational and electronic properties of small molecules on metal surfaces YANNING ZHANG, CHEN XU, CHI-LUN JIANG, WILSON HO, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, CA 92697 — Research of manipulating chemical bonds in a single molecule has been extremely active in recent years. Using a newly built milli-Kelvin scanning tunneling microscope, we can now resolve vibrational spectroscopic features down to a few tenths meV. Synergistic density functional calculations allow correct interpretation for each vibrational mode and provide links between experimental observations to the change of individual chemical bonds. In particular, we explored the effect of tunneling gap distance on different vibrational energies, by moving the tip toward the molecules, so as to shed some light for selective bond dissociation and formation. Here we discuss our results of the atomic structure, vibrational and electronic properties of several small molecules such as CO on the anisotropic Au(110) surface and C₂H₂ on the Cu(001) square lattice. Calculated vibrational frequencies, using the generalized gradient approximation or the non-local van der Waals density functional, are in good agreement with experimental results. **Acknowledgement.** Work was supported by the National Science Foundation under CHE-0802913 and computing time at XSEDE.

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