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Bond dissociation of small molecules on the silver tip under the influence of local electric field HAIYAN HE, Department of Physics and Astronomy, University of California, Irvine, CA 92697, MAYUKH BANIK, VARTKESS APKARIAN, Department of Chemistry, University of California, Irvine, California 92697, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, CA 92697 — The manipulation of chemical bonds at metallic nano-junctions, such as at scanning tunneling junctions, and under laser irradiation is currently of great interest, motivated by both fundamental considerations and applications in nanoeletronics, nanophotonics and nanocatalysis. In this work, we systematically investigate bond formation and dissociation of small molecules (e.g., oxygen and carbon monoxide) at the junction of two silver (111) tipped surfaces, through first principles molecular dynamics simulations. The electronic structures and vibrational frequencies are a sensitive function of the gap size, and significantly modified by the local electric fields. The calculated results are compared with recent experiments. **Acknowledgement.** This work was supported by the National Science Foundation under CHE-0802913 and computing time at XSEDE.

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