Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

First-principles study of surface stresses induced by target-receptor interactions on a cantilever sensor VARADHARAJAN SRINIVASAN, Computational Nanoscience Group, Univ. of California, Berkeley, GIANCARLO CICERO, Dept. of Physics, Polytechnic of Torino, JEFFREY C. GROSSMAN, Computational Nanoscience Group — Nanoscale cantilevers have shown great promise as ultrasensitive, low-power chemical sensors based on the surface stresses induced by interactions between the target species and the receptor coating layer. However, the basic mechanism of these induced stresses is yet to be fully understood, and it is therefore of great fundamental and practical interest to elucidate their electronic and structural origins via the weak interactions that lead to cantilever deflection. An example of such a device is the Au-SiN_x cantilever sensor using functionalized long-chain alkanethiols as a coating layer. Even though the target-receptor interactions are often weak, the induced stresses are quite sensitive to the chemistry of the interacting species. Taking water molecules as a model target and ω-hydroxy and ω-carboxy alkanethiols as the receptor layer on a Au(111) surface, we use first-principles surface stress calculations to provide a detailed atomistic-level understanding of the various contributions leading to the deflection of a cantilever.

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Date submitted: 27 Nov 2007 Electronic form version 1.4