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Chain-length dependence in surface stresses of alkanethiolate-covered Au(111)[1] V. SRINIVASAN, Berkeley Nanoscience and Nanoengineering Institute, UC Berkeley, CA 94720, G. CICERO, Materials Science and Chemical Engineering Department, Politecnico of Torino, C.so Duca degli abruzzi 24, 10129, Torino, Italy, J. C. GROSSMAN, Berkeley Nanoscience and Nanoengineering Institute, UC Berkeley, CA 94720 — We have recently shown [2] that adsorption-induced stresses in alkanethiolate-covered Au(111) contribute significantly to the stress-response in nano-mechanical cantilever sensors. In particular, we proposed a local stress relief (LSR) mechanism whereby charge removal by the Au-S bond from the Au surface promotes a stress reducing rearrangement of surface Au atoms. Since LSR depends on the nature of the Au-S bond it was unclear how the contribution to the stress- response would depend on the alkanethiolate structure. We present a first-principles study of the chain-length dependence in surface stresses of alkanethiolate-covered Au(111). We find that the surface stress upon adsorption is anisotropic and tensile, increasing in magnitude with the chain-length. We analyze this trend in the context of the LSR mechanism and inter-adsorbate interactions.

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[2]Phys. Rev. Lett. **101**, 185504 (2008)

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