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Calibrating the Bending of Molecule Adsorbed Nanoscale Si Cantilevers with a Modified Stoney Formula¹ JI ZANG, FENG LIU, Department of Materials Science and Engineering, University of Utah, Salt Lake City, UT 84112 — Fundamental understanding of mechanical bending of molecule adsorbed nanoscale thin films is of both scientific and technological importance. Our current understanding, however, is limited within macroscopic analysis that neglects the atomic details of film structure and surface effects. Here, we report atomistic simulation and theoretical analysis of bending of freestanding nanometer-thick silicon (Si) films induced by adsorption of hydrogen and acetylene molecules. It reveals the dominant role of atomic surface structure and surface stress in governing their bending behavior. We show that the bending curvature of molecule adsorbed Si nanofilm does not follow the classical Stoney formula, and we develop a modified Stoney formula by taking into account of the effects arising from atomic surface reconstruction and surface stress. Our findings suggest that re-calibration has to be made in detecting trace amount of molecules by nanoscale Si mechanochemical sensors.

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