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Vibrational spectrum and stability of the long-debated models for the $(\sqrt{7}\times\sqrt{7})R19\circ$ phase of S/Cu(111)[1] MARISOL ALCANTARA ORTIGOZA, MARAL AMINPOUR, TALAT S. RAHMAN, University of Central Florida — Recently, the structure of the copper sulfide overlayer formed on Cu(111) upon sulfur exposure has attracted attention because it serves as a substrate to form MoS_2 monolayers and MoS_X nanostructures in a controlled manner, which may have numerous technological applications. In the past, at least eight experimental techniques have been used to characterize the $(\sqrt{7}\times\sqrt{7})R19\circ$Cu-S overlayer on Cu(111) and to support or refute a large number of possible models but, as yet, at least three models are still in dispute. In this study, we provide firmer arguments to resolve the structure of CuS/Cu(111) at the atomic scale. Specifically, we perform density-functional-theory calculations of the total energy and the vibrational spectrum of the proposed structures to (1) attest their dynamical stability; (2) compare their thermodynamic stability as obtained from the total free energy; and (3) provide the vibrational frequencies that uniquely fingerprint these structures and which may serve for further experimental confirmation or refutation.

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