Electronic structure of the indium-adsorbed Au/Si(111)-\(\sqrt{3} \times \sqrt{3}\) surface: a first-principles study

FENG-CHUAN CHUANG, CHIA-HSIU HSU, WEN-HUAN LIN, Department of Physics, National Sun Yat-sen University, Taiwan, VIDVUDS OZOLINS, Department of Materials Science and Engineering, University of California, Los Angeles, Los Angeles, CA 90095-1595, USA — Electronic structures of the indium-adsorbed Au/Si(111)-\(\sqrt{3} \times \sqrt{3}\) surface were examined using first-principles calculations at In coverages range from 0.15 ML to 1 ML. The band structures of the various proposed models were analyzed in detail. Our results show that the calculated bands for the identified atomic models for indium-adsorbed on conjugate honeycomb-chained-trimer model at In coverages of 1/3 ML and 2/3 ML are in agreement with the identified bands in the angle-resolved photoemission study [Phys. Rev. B 80 075312 (2009)].