Abstract Submitted
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Insights on the electronic and vibrational properties of Bi(111) from first principles[1] MARISOL ALCANTARA ORTIGOZA, ROLF HEID, KLAUS-PETER BOHNEN, Karlsruhe Institute for Technology, IRINA SKLYADNEVA, Donostia International Physics Center, NEHA NAYYAR, TALAT S. RAHMAN, University of Central Florida, EUGENE CHULKOV, Donostia International Physics Center — Bi(111) is known to have surface electron carriers close to Γ as well as hole carriers at Γ and along the ΓM directions. The lattice dynamics of Bi(111) is however largely unknown. We investigate both the electronic structure and lattice dynamics of Bi(111) films via density-functional-theory and density-functional-perturbation-theory calculations taking into account the spin-orbit coupling (SOC). While the splitting of the branches is dominated by the SOC almost everywhere along the ΓM direction, around the zone boundary (M), the delocalized character of this state plays an important role. Reducing the thickness of a film decreases the band gap progressively. At ∼3-nm thickness, the highest valence band re-crosses the Fermi level and creates extra electron pockets. We find, however, that the lattice dynamics of Bi(111) is robust with respect to film thickness. Bi(111) has a number of "high-lying" surface modes in the optical band almost everywhere along the ΓKM and ΓM directions, most notably, a vertical mode slightly above the bulk band. Surface acoustic modes are also present as well as some "low frequency" optical modes in small regions of the zone. A comparison with recent measurements will be presented, as well as the possible implications on the electron-phonon coupling.

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