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First-Principle Calculations and Raman Studies of Surface Phonons in the Topological Insulators Bi_2Se_3 and Bi_2Te_3. IBRAHIM BOULARES, GUANGSHA SHI, CTIRAD UHER, EMMANOUIL KIOUPAKIS, ROBERTO MERLIN, U. Michigan, PETR LOSTAK, U. Pardubice - Czech Republic — Raman [1-2], helium scattering [3] and photoemission experiments [4] on the topological insulators Bi_2Se_3 and Bi_2Te_3 show features in the range ˜50-150 cm-1, which have been assigned to Raman-forbidden, infrared modes due to symmetry breaking at the surface [1-2] or surface phonons [3,4], which couple to the topologically protected electronic states [4]. We present first-principle LDA calculations and temperature-dependent Raman studies showing strong evidence of the existence of surface phonons in both Bi_2Se_3 and Bi_2Te_3. The calculations reveal that these modes are quite insensitive to spin-orbit coupling, an indication that their occurrence is unrelated to the topological properties of these materials. [1] K. M. F. Shahil et al., Appl. Phys. Lett. 96, 153103 (2010). [2] V. Gnezdilov et al., Phys. Rev. B 84, 195118 (2011). [3] X. Zhu et al., Phys. Rev. Lett. 107, 186102 (2011). [4] J. A. Sobota et al., Phys. Rev. Lett. 113, (2014).

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