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First-principles exploration of high-energy facets of bismuth chalcogenide nanocrystals[1] OLEG V. YAZYEV, NAUNIDH VIRK, Ecole Polytechnique Federale de Lausanne (EPFL), Switzerland — Binary bismuth chalcogenides Bi_2Se3, Bi_2Te_3, and derived materials are currently considered as the reference topological insulators (TIs) due to their simple surface-state band structures and relatively large bulk band gaps. Nanostructures of TIs are of particular interest as a large surface-to-volume ratio enhances the contribution of surfaces states. So far, the vast majority of research efforts have focused on the low-energy (111) surfaces which correspond to weak planes in the layered crystal structures. Low-dimensional nanostructures such as nanowires and nanoparticles will inevitably involve higher energy facets. We perform a systematic ab initio investigation of the high-energy surfaces of bismuth chalcogenide TIs characterized by different crystallographic orientations as well as surface reconstructions and stoichiometries. We find several stable surfaces which exist under varying thermodynamic equilibrium conditions. Surface orientation and stoichiometry are found to dramatically affect band dispersion and spin polarization of the topological surface-state charge carriers.

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