ABSTRACT

Title of Document	**Surface study of Cu₂SnS₃ using first principle density functional theory**
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In this work, the electronic structure of Cu_2SnS_3 (CTS) along with the surface energy and surface electronic structure are computed using density functional theory (DFT). Here the monoclinic phase is considered for computing the electronic structure of the bulk CTS, whereas (200) and ($\bar{1}$31) terminated surfaces from bulk CTS are considered for the surface energy calculation. Here the electronic structure of the bulk and surface CTS are calculated using the Heyd–Scuseria–Ernzerhof (HSE) screened hybrid density functional after geometry optimization of ions by a Local Density Approximation (LDA). Moreover, the valence band (VB) in bulk CTS is found to composed of mainly Cu 3d orbital along with the minor contribution of S 3p orbital, whereas, the conduction band (CB) is found to primarily consist of S 3p along with a minor contribution from Sn 5s states. Surface distortion is seen on both these considered CTS surfaces after geometrical optimization of these supercells in which both these surfaces undergo ionic relaxation. In (200) surface supercell, Cu and Sn atoms are seen to move inwards,

and outwards respectively, whereas, for ($\bar{1}$31) surface supercell, S atoms show high lateral displacement. Moreover, the surface energy of (200) and ($\bar{1}$31) surfaces are calculated to be 0.0234 and 0.174 eV/Å^2, respectively, indicating (200) being the most stable CTS surface. In addition, the influence of surface relaxation on the electronic surface structure of each of these surfaces is investigated through the partial state density (PDOS), which results in an overlap of VB and CB for both these surfaces, implying these surfaces being metallic. Finally, the relaxation effect on the subsurface atoms is studied, which resulted in the displacement of the subsurface ions of the order of less than 0.1 Å, this further reduced beyond the second layer.