

Abstract Submitted  
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**Wurtzite-derived polytypes of kesterite and stannite quaternary chalcogenide semiconductors** SHIYOU CHEN, Lab of Polar Materials and Devices, East China Normal University, YE LUO, XIN-GAO GONG, Fudan University, ARON WALSH, University College London, SU-HUAI WEI, National Renewable Energy Lab — The  $I_2-II-IV-VI_4$  quaternary chalcogenide semiconductors (*e.g.*,  $Cu_2ZnSnS_4$ ,  $Cu_2ZnGeSe_4$ ) have been studied for more than 40 years, but the nature of their crystal structures has proved contentious. Literature reports exist for the stannite and kesterite structures, which are zincblende-derived structures, and wurtzite-stannite, which is a wurtzite-derived structure. In this talk we report a new wurtzite-derived structure, wurtzite-kesterite (space group  $Pc$ ), which is the ground state for some  $I_2-II-IV-VI_4$  compounds, but is easily confused with the wurtzite-stannite structure. We show that there is a clear relationship between the properties of the wurtzite-kesterite and zincblende-derived kesterite structures, as well as between wurtzite-stannite and stannite. The energy stability of different structures are studied according to the strain and Coulomb energy contributions, showing a dependence on the size and ionicity of the component atoms. Electronic structure of the wurtzite-derived structures will also be discussed.

Shiyu Chen  
Lab of Polar Materials and Devices, East China Normal University

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