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Hybrid Functional Study of Sodium and Potassium Incorporation in Cu_2ZnSnS_4[1] KIN FAI TSE, MANHOI WONG, YIOU ZHANG, JINGZHAO ZHANG, JUNYI ZHU, Chinese Univ of Hong Kong — The thermodynamics of Na and K incorporation and its effects in Cu2ZnSnS4 (CZTS) is studied using density functional theory with hybrid functional. The allowed chemical potential of Na/K in CZTS is established. Formation energy calculations shows that Na can be significantly incorporated as both substitutional defects and interstitial defects, and incorporation of K related defects are generally less favorable. Transition energy calculations is performed showing that both Na and K exhibit benign defect properties and act as a p-type dopant. The qualitative disagreement between GGA with rigid band edge shifting and HSE calculations, formation of defect complexes, and implications in experiment will also be discussed. The understandings on the defect properties of Na and K provides an essential knowledge to further understand the surfactant effects of Na and K observed in experiments.

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