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Metal Disorder in Cu_2ZnSnS_4 (CZTS) Solar Cells from Multi-Scale Simulations SUZANNE WALLACE, JARVIST FROST, ARON WALSH, University of Bath — Kesterite-structured Cu_2ZnSnS_4 (CZTS) is a promising earth-abundant and non-toxic material for the active layer of thin-film solar cells due to its high optical absorption coefficient of $> 10^4$ cm^{-1} and sunlight matched band gap of 1.5 eV. Device efficiencies are hampered by low open circuit voltage (V_{OC}) compared to the optical band gap. One possible origin of this is disorder amongst the Cu and Zn ions. Such disorder could lead to sub band-gap recombination centres due to fluctuations in electrostatic potential from the presence of charged defects. Understanding the origin of these sub-gap states, and the resulting impediment on device performance, is essential to discover design and processing rules for high efficiency kesterite, and other multi-component semiconductor, devices. We investigate this by writing custom Monte-Carlo codes to simulate the on-lattice disorder. A generalised Ising Hamiltonian is parameterised with hybrid density functional theory (DFT) total-energy calculations on defect pairs. The resulting disorder is simulated as a function of temperature, and the order-disorder behaviour and resulting local and long-range electrostatic potential variation due to Cu-Zn disorder is quantified.

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