## Abstract Submitted for the MAR17 Meeting of The American Physical Society

First principles investigation of the structural, dynamical, dielectric properties of kesterite, stannite and PMCA phases of Cu<sub>2</sub>ZnSnS<sub>4</sub> SRIRAM POYYAPAKKAM RAMKUMAR, YANNICK GILLET, ANNA MIGLIO, MICHIEL J. VAN SETTEN, XAVIER GONZE, GIAN-MARCO RIGNANESE, Univ Catholique de Louvain — Cu<sub>2</sub>ZnSnS<sub>4</sub> (CZTS) is a promising material as an absorber in photovoltaic applications. The measured efficiency, however, is far from the theoretically predicted value for the known CZTS phases. To improve the understanding of this discrepancy we investigate the structural, dynamical, and dielectric of the three main phases of CZTS (kesterite, stannite, and PMCA) using density functional perturbation theory (DFPT). The effect of the exchange-correlation functional on the computed properties is analyzed. A qualitative agreement of the theoretical Raman spectrum with measurements is observed. However, none of the phases correspond to the experimental spectrum within the error bar that is usually to be expected for DFPT. This corroborates the need to consider cation disorder and other lattice defects extensively in this material.

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