Abstract Submitted
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Electron and Phonon Properties of Type II Sn Clathrates via First Principles Methods.[1] ARTEM KHABIBULLIN, KAYA WEI, University of South Florida, HUAN TRAN, University of Connecticut, GEORGE NOLAS, LILIA WOODS, University of South Florida — Clathrates are cage-like materials where high carrier mobility can coexist with low thermal conductivity. Much of the work to date has focused on the role of the guest atoms inside type I clathrate framework. The rattling of the guest atoms inside the clathrate voids is an effective way to reduce the lattice thermal conductivity leading to enhancing the figure of merit of a thermoelectric material. The focus of our investigation are type II Sn clathrates, which have been explored to a lesser extent as compared to Si or Ge materials. We present results from density functional theory simulations for calculated lattice structure, electronic structure and phonon dynamics properties. Our comprehensive investigation shows that the type of guest atoms and cage substitution via Ga atoms strongly affect the energy band structure coupled with anharmonicity effects originating from the guest atoms. Unusual effects arising from weak van der Waals interactions and important signatures in the Gruneisen parameters have also been identified. Our study expands upon the fundamental understanding of clathrate materials as new pathways for property modifications are presented.

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