

Abstract Submitted
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Vibrational Dynamics of Filled Skutterudites SUSMITA BASAK, CHRISTIAN CARBOGNO, MATTHIAS SCHEFFLER, Fritz Haber Institute of the Max Planck Society — Skutterudites are promising candidates for thermoelectric applications, since their cage like structure can be filled with guest atoms to tune the electronic and vibrational properties and so to optimize the thermoelectric transport coefficients. Various conflicting phenomenological models (e.g., incoherent rattling, coherent coupling [1]) have been proposed to explain the interaction between guest and host, but the exact mechanisms are still topic of debate. To clarify this question, we determine the temperature dependence of the geometric, electronic, and vibrational properties for a set of skutterudites (CoSb_3 , CoAs_3) and guests (Ga, In, Sn, etc.) using density-functional theory in the quasi-harmonic approximation. We find different coupling mechanisms to be active depending on the guest, which leads to drastically different dynamics ranging from localized to coherent phonon modes. These modes, which are robust against doping and defy the common assumption that the guest's mass primarily determines the coupling, also largely influence the structural and electronic properties. Finally, we discuss the implications of our findings for the control and optimization of the thermoelectric efficiency. [1] M. M. Koza *et al.*, Nat. Mat. **7**, 805, (2008).

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