Abstract Submitted
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Ab initio calculations of intrinsic defects in ZnSb LASSE BJERG, Aarhus University & Massachusetts Institute of Technology, GEORG K.H. MADSEN, Ruhr-Universität Bochum, JEFFREY C. GROSSMAN, Massachusetts Institute of Technology, BO B. IVERSEN, Aarhus University — Thermoelectric materials are capable of interconverting heat and electricity. The most efficient thermoelectric materials are heavily doped semiconductors, and hence they can be either n- or p-type. ZnSb has recently been predicted by theoretical calculations to be a good n-type thermoelectric material. However, synthesis produces p-type materials. Intrinsic point defects have been investigated as a possible origin using ab initio calculations. Negatively charged Zn vacancies are found to have a low formation energy, and an intrinsic p-type behavior is predicted.

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