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First-principles study of thermoelectric properties of pyrite YI XIA, Department of Materials Science and Engineering University of California, Los Angeles, FEI ZHOU, Lawrence Livermore National Laboratory, VIDVUDS OZOLINS, Department of Materials Science and Engineering University of California, Los Angeles — Due to its natural abundance, moderate band gap and good light absorption properties, pyrite (FeS_2) is being considered for use in nanocrystalline solar cells. High-quality n-type samples show high electron mobility, but their adoption in solar cells is hampered by low open circuit voltages. Here, using density-functional theory (DFT), we study charge and thermal transport properties of FeS_2. Using the Debye-Callaway model, we obtain lattice thermal conductivity in good agreement with experimental data, suggesting that significant reduction of lattice thermal conductivity would be needed for thermoelectric applications. In addition, we find that holes in p-type pyrite form localized small polaron states, which naturally explains low hole mobilities observed experimentally.

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