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Quasiparticle band structures and thermoelectric transport properties of Mg_2Si, Mg_2Ge, and Mg_2Sn[1] GUANGSHA SHI, EMMANOUIL KIOUPAKIS, Materials Science and Engineering, University of Michigan — Mg_2Si, Mg_2Ge, and Mg_2Sn are narrow-gap semiconductors with large Seebeck coefficients and favorable thermoelectric properties. We calculated the quasiparticle band structures of Mg_2Si, Mg_2Ge, and Mg_2Sn using density functional and many-body perturbation theory in the GW approximation. The calculated band gaps are in good agreement with experiment. The inclusion of semicore states in the valence is necessary to obtain accurate band gaps for Mg_2Ge and Mg_2Sn. We used the maximally localized Wannier function method and the Boltzmann transport equation in the constant relaxation-time approximation to determine the Seebeck coefficient and the electrical and carrier thermal conductivities. We discuss the importance of quasiparticle corrections to accurately determine the Seebeck coefficients at high temperatures.

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