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Thermoelectric properties of higher manganese silicides[1] YU-CHIH TSENG, Natural Resources Canada, VIJAY SHANKAR VENKATARAMAN, HAE-YOUNG KEE, University of Toronto — Higher manganese silicides (HMS) are promising thermoelectric materials that may be broadly deployable because of the abundance of the constituent elements and their non-toxic nature. We study the thermoelectric properties of HMS using density functional theory calculations and tight-binding models to fit these calculations. We estimate charge carrier density and mobility, and compare with experimental data. Theoretically obtained thermal and electrical conductivities, and the Seebeck coefficients are presented. Possible scattering mechanisms and relations to figure of merit are also discussed.

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