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Thermoelectric properties of titanium dioxide polymorphs from first principles DYLAN BAYERL, EMMANOUIL KIOUPAKIS, University of Michigan - Ann Arbor — Titanium oxides are promising materials for high-temperature thermoelectrics because of their high Seebeck coefficients, thermal stability, and natural abundance. We use first-principles calculations to investigate the thermoelectric transport properties of several titanium dioxide polymorphs. Our methodology is based on density functional and many-body perturbation theory within the GW approximation. The maximally localized Wannier function method is employed to interpolate the GW bands in the Brillouin zone. We use the Boltzmann transport formalism within the constant relaxation time approximation to determine the temperature and carrier-density dependence of the Seebeck coefficient, electron mobility, and electron thermal conductivity from the calculated electronic band structures. We demonstrate agreement with experimentally measured transport parameters and enhanced power factor at high temperature in certain heavily doped phases. This research was supported as part of CSTEC, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science. Computational resources were provided by the DOE NERSC facility.

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