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Thermoelectric properties of ZnO under high pressure: a first-principles study ANDREW ALVARADO, JEEVAKE ATTAPATTU, YI ZHANG, CHANGFENG CHEN, Department of Physics and Astronomy and High Pressure Science and Engineering Center, University of Nevada, Las Vegas — ZnO is a very important semiconducting material that exhibits interesting physical properties with great promise for applications in electronic and optical devices. A recent study predicted that ZnO may be a viable high-temperature thermoelectric material at ambient pressure. There is, however, a lack of understanding of the thermoelectric properties of its high pressure phases. Here we report our first-principles studies of thermodynamic and thermoelectric properties of wurtzite, zinc-blended, and rocksalt phases of ZnO. Using the Boltzmann transport theory, we obtained the dependence of the figure of merit ZT on doping and temperature. Our results establish the quenchable high-pressure ZnO phase as a promising high-temperature thermoelectric material.

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