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Enhancing thermoelectric power factor with highly mismatched isoelectronic doping JOO-HYOUNG LEE, Massachusetts Institute of Technology, JUNQIAO WU, University of California, Berkeley, JEFFREY GROSSMAN, Massachusetts Institute of Technology — With a view to enhancing the thermoelectric Seebeck effect by introducing highly electronegativity mismatched impurities, we investigate the effect of O impurities on the thermoelectric properties of ZnSe from a combination of first-principles and analytic calculations. It is demonstrated that dilute amounts of O impurities introduce peaks in the density of states (DOS) above the conduction band minimum, and that the charge density near the DOS peaks is substantially attracted toward O atoms due to their high electronegativity. The impurity-induced peaks in the DOS result in an increase of the room-temperature Seebeck coefficient and power factor from those of O-free ZnSe by a factor of 30 and 180, respectively. Other impurities with different electronegativities such as N-F dual impurities and S are also examined and it is found that this effect is absent when the impurity electronegativity well matches the host that it substitutes. The results suggest that highly electronegativity-mismatched alloys can be designed for high performance thermoelectric applications.

Joo-Hyoung Lee
Massachusetts Institute of Technology

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