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Thermoelectric properties of amorphous ZnO-based materials using *ab initio* methods ANINDYA ROY, YU-TING CHENG, MICHAEL L. FALK, Johns Hopkins Univ — We use a combination of computational methods - molecular dynamics and density functional theory, to predict thermoelectric properties of amorphous ZnO-based materials. We use BoltzTraP [1] to calculate properties such as Seebeck coefficient and electrical conductivity within semiclassical Boltzman transport theory, and compare with available experimental results. Additionally, we investigate the change in the thermoelectric parameters caused by alloying amorphous ZnO with tin and other elements. Our preliminary calculations suggest that the thermoelectric performance of amorphous ZnO is on par with the crystalline counterpart. This is encouraging - since amorphous materials are yet to be studied in depth for their potential as thermoelectric materials, and they could see much improvement with sustained effort. Also, while *ab initio* methods are routinely used to predict properties of crystalline systems, their application in amorphous systems is a less-explored area.

[1] BoltzTraP: Madsen, G. K. and Singh, D. J., Comput. Phys. Commun. **175**, 67-71 (2006).

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