Thermoelectric performance in ultra-thin transition metal dichalcogenides\(^1\) DARSHANA WICKRAMARATNE, University of California - Riverside, FERDOWS ZAHID, The University of Hong Kong, Hong Kong SAR, China, ROGER LAKE, University of California - Riverside — The thermoelectric figure of merit, ZT, is calculated for one to four monolayers of MoS\(_2\), MoSe\(_2\), WS\(_2\) and WSe\(_2\). The maximum ZT in this family of materials occurs in bilayer MoSe\(_2\). Its ZT value of 2.39 is a factor of 8 increase compared to that of the bulk at room temperature. The values for the power factors and ZT change non-monotonically as the film thicknesses are increased from a single monolayer up to four layers. In contrast to Bi\(_2\)Te\(_3\), the peak value of ZT occurs at a thickness greater than a single monolayer for all 4 materials. The shape of the distribution of the valence band and the conduction band density of modes explains the enhanced thermoelectric performance that occurs for film thicknesses above a single monolayer. Ab-initio electronic structure calculations are used in a Landauer approach to calculate the thermoelectric transport coefficients.

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