Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

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_2Te_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.

[1]NSF and SRC-NRI project 2204.001 (NSF-1124733), FAME, one of six centers of STARnet, a SRC program sponsored by MARCO and DARPA. This work used the XSEDE which is supported by the NSF grant number OCI-1053575

Darshana Wickramaratne
University of California - Riverside

Date submitted: 15 Nov 2013 Electronic form version 1.4