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Directed phonon engineering in nanostructured Mn-Ge superlattices: Towards a description of heat transport in device-like structures[1]

CLAUDIA MANGOLD, Max Planck Institute for Polymer Research, Germany, JOERG BEHLER, Ruhr University Bochum, Germany, DAVIDE DONADIO, Max Planck Institute for Polymer Research, Germany — Poor performance of thermoelectric materials severely limits the application of Peltier devices. Our work aims at the improvement of the efficiency of such devices by replacing standard p-n junctions with a membrane structure with nanofeatures. The low dimensionality of the membranes and the nanofeatures will ensure a reduction of the phononic thermal conductivity κ, thus enhancing the thermoelectric figure of merit, $ZT=S^2\sigma T/\kappa$. Mn-Ge compounds turned out to be excellent candidates for nanostructuring due to the broad structural variety[1]. We performed first-principles electronic structure calculations, in particular density functional theory, to characterize various Mn-Ge bulk species as well as Mn-Ge superlattices. To reach larger length scales we have constructed a transferable neural network potential[2] for Mn-Ge compounds to characterize nanostructured membranes up to device-like size and determine their thermal transport properties. This multiscale modeling approach is a powerful tool to design materials and devices with specifically engineered phonon properties and enhanced thermoelectric performances. [1]Jamet et al Nature Mat.5,653(2006);Jain et al J.Appl.Phys. 109,013911(2011) [2]Behler et al PRL 98,146401(2007);Phys.Stat.Sol.B 245,261(2008)

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