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**Doping dependence of thermoelectric performance in $Mo_3Sb_7$: first principles calculations**[1] DAVID PARKER, MAO-HUA DU, DAVID SINGH, Oak Ridge National Laboratory — Experimental studies have indicated the substantial thermoelectric promise of doped $Mo_3Sb_7$, with a figure-of-merit ZT of 0.9 (H. Xu *et al*, J. Appl. Phys. **105**, 053703 (2009)) already achieved at high temperature. However, optimal doping levels have not yet been achieved. We study doping of $Mo_3Sb_7$ with transition metals (Ni,Fe,Co,Ru) via first principles calculations, including electronic structure, lattice dynamics and Boltzmann transport. We discuss the selection of dopant and the potential thermoelectric performance of optimally doped $Mo_3Sb_7$.

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