Novel Te-bearing half-Heusler phases and their potential thermoelectric performance

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Theoretical predictions from first principles were conducted on nine half-Heusler tellurides ($M^{IV}M^{VIII}Te$, where M^{IV} = Ti, Zr, Hf, and M^{VIII} = Fe, Ru, Os), each possessing 18 valence electrons. Among the compounds investigated, eight were found to be novel and mechanically stable according to the Born criteria for elastic constants. The MBJGGA approach predicted eight of the examined compounds to be semiconductors, with band gaps ranging from 0.395 eV (ZrOsTe) to 1.247 eV (ZrRuTe). Detailed analysis was conducted on the band gaps, spin-orbit splitoffs of heavy- and light-hole bands, elastic constants, and effective masses in the half-Heusler tellurides. Chemical trends were observed for the transition metal ions considered, with Fe-bearing compounds exhibiting the widest band gaps. The compounds ZrOsTe and HfRuTe are expected to have potential applications in thermoelectric devices due to Mahan's '10 k_B T rule'. The thermoelectric performance was discussed based on transport calculations, the deformation potential theory approximation for the relaxation time of carriers, and Slack's approximation for the lattice thermal conductivity. ZT (figure of merit) values as high as 2.76 and 4.14 at 1100 K were predicted for ZrOsTe and HfRuTe, respectively. This comprehensive investigation of half-Heusler tellurides presents interesting systems for further experimental research.

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