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Electronic and Thermoelectric Properties of Zintl 14-1-11 Compounds Computed with DFT+U TRINH VO, PAUL VON ALLMEN, SABAH BUX, JEAN-PIERRE FLEURIAL, JPL/CalTech — We present results for the electronic structure and thermoelectric properties of zinlt 14-1-11 compounds, in particular Ca14-yYbyAlSb11-xAsx (x = 0.11, and y = 0.14) and Yb14MgSb11, using DFT+U and Boltzmann's transport equation. The effect of selective substitutions at different cation, anion, and central metal sites on the electronic properties is also investigated. We found that selective atomic substitution affects the electronic structure significantly, leading in certain cases to substantial improvement of the thermoelectric properties.

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