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# Theoretical investigation of ternary semiconductors half-Heusler RhTaZ (Z = Si, Ge and Sn) for thermoelectric applications

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The structural, electronic, elastic, thermodynamic and thermoelectric properties of RhTaZ (Z = Si, Ge and Sn) half-Heusler materials have been studied using density functional theory. We have found that the compounds studied can be experimentally synthesized. Also, RhTaZ (Z = Si, Ge and Sn) alloys exhibit a semiconductor behavior following the Slater–Pauling rule. The elastic properties calculated confirm that our compounds are mechanically stable. Using Debye's quasi-harmonic model, the thermodynamic properties of these half-Heusler alloys were investigated. For the study of thermoelectric properties, the semi-classical Boltzmann theory, as implemented in the BoltzTraP code, has been used. The high values obtained from the figure of merit for RhTaZ (Z = Si, Ge and Sn) compounds suggest that they are promising candidates for thermoelectric applications at low and high temperatures.

*Keywords*: Half-Heusler; density functional theory (DFT); semiconductor behavior; thermodynamic and thermoelectric properties.

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