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Evolutionary structure search of efficient thermoelectric compounds MARIBEL NÚÑEZ VALDEZ, Moscow Institute of Physics and Technology, ARTEM OGANOV, Skolkovo Inst Sci and Tech; Moscow Inst of Phys and Tech; SUNY Stony Brook, Dept Geosci Ctr Mat Design; SUNY Stony Brook, Inst Adv Computat — Thermoelectric materials, which are used to harvest waste heat to generate power, are taking an important role for energy solutions. However, it is of fundamental significance the optimization of a variety of conflicting properties in order to obtain a high efficiency thermoelectric device to be cost-effective for applications. This efficiency or figure of merit (ZT), which depends on the Seebeck coefficient, electrical resistivity and heat conductivity, is restricted by currently available materials and fabricating technologies. Therefore, the main objective of our study is the identification of thermodynamically stable compounds and their crystal structures with high ZT given just a set of elements by using an evolutionary algorithm in which the figure of merit is a degree of freedom to be optimized. We test the performance of our methods within the system Bi_2Te_3-Sb_2Te_3. These compounds are well known for their large ZT's and their use in technological applications. Our results indicate a high feasibility for the employment of our evolutionary algorithm search using a wide variety of elements for optimizing and designing new thermoelectric materials.

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