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Thermoelectric properties of low-dimensional clathrates from first principles DEEPA KASINATHAN, HELGE ROSNER, MPI CPfS — Type-I inorganic clathrates are host-guest structures with the guest atoms trapped in the framework of the host structure. From a thermoelectric point of view, they are interesting because they are semiconductors with adjustable bandgaps. Investigations in the past decade have shown that type-I clathrates $X_8Ga_{16}Ge_{30}$(X = Ba, Sr, Eu) may have the unusual property of "phonon glass-electron crystal" for good thermoelectric materials. Among the known clathrates, $Ba_8Ga_{16}Ge_{30}$ has the highest figure of merit (ZT 1). To enable a more widespread usage of thermoelectric technology power generation and heating/cooling applications, ZT of at least 2-3 is required. Two different research approaches have been proposed for developing next generation thermoelectric materials: one investigating new families of advanced bulk materials, and the other studying low-dimensional materials. In our work, we concentrate on understanding the thermoelectric properties of the nanostructured Ba-based clathrates. We use semi-classical Boltzmann transport equations to calculate the various thermoelectric properties as a function of reduced dimensions. We observe that there exists a delicate balance between the electrical conductivity and the electronic part of the thermal conductivity in reduced dimensions. Insights from these results can directly be used to control particle size in nanostructuring experiments.

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