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Structural, electronic and thermal properties of Sn clathrates

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**Abstract content (Max 300 words)
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Sn clathrates are promising “phonon glass, electron crystal” materials[1], in which the phonon free paths are short and the electron free paths are long. We analysed the relaxed structure of Sn clathrates using four different Density Functional Exchange-Correlation functionals. The phonon structures were investigated as a first in the effort to determine the phonon contribution to the thermal conductivity. We determined the Seebeck coefficient and electrical conductivity of the clathrate compound and the Thermo Electric figure of merit. A peep into the dynamics of the system for the evaluation of the thermoelectric and electronic properties is presented.

[1]Slack, G.A. , 1995, in CRC Handbook of Thermoelectrics, edited by D.M. Rowe (CRC Press, Boca Raton, FL), pp. 407-440

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