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Thermoelectric Transport Properties of Hypothetical Type-VIII Clathrate Si_{46} PAYAM NOROUZZADEH, Oklahoma State Univ, CHARLES MYLES, Texas Tech University, DARYOOSH VASHAEE, Oklahoma State Univ — Our first principles calculations on hypothetical type-VIII clathrate Si_{46} [1] revealed that it has a large density of states near the band edges which can result in large thermoelectric power factor. The large number of valleys around the valance band edge can improve the performance of p-type thermoelectric material. The calculated thermoelectric transport properties using multiband Boltzmann transport equation and the data from density functional theory and molecular dynamics simulations are presented for the bulk crystalline and the effect of nanostructuring is investigated as well. The predicted figure-of-merit of bulk nanostructured p-type Si_{46}-VIII clathrate is in the order of 2 at 1000 C. The InfraRed and Raman active modes are identified which will be especially useful for the experimental characterizations of this material.

[1] Payam Norouzzadeh *et al* 2013 *J. Phys.: Condens. Matter* **25** 475502

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