Dear Editor,

We would like to submit our manuscript entitled “The intrinsic low lattice thermal conductivity in the rock salt SnSe” for the publication as a regular paper in computational materials science.

An exciting discovery is that the orthorhombic Tin Selenide (SnSe) shows extremely low lattice thermal conductivity () and thus achieves a record high zT value. Since most other IV-VI thermoelectric materials adopt the high symmetry rock salt structure, it is very desirable to know whether such low thermal conductivity is from the orthorhombic structure, if the rock salt SnSe would have even smaller thermal conductivity.

In the present manuscript, based on first principles calculations and the Boltzmann transport equation, we have identified an even lower for the rock salt SnSe. We carefully studied the thermal transport properties for both the orthorhombic SnSe and the rock salt SnSe. We attributed the low of the rock salt SnSe to its large Grüneisen parameters, which stem from the strongly anharmonic phonons. This anharmonic effect is further confirmed by the prominent long-range force constants in the rock salt SnSe. The of the rock salt SnSe is mostly contributed to by the optical phonons, which would be effectively reduced further if the optical contributions are eliminated by defects in experiments.

This comparative study of the rock salt and orthorhombic structured SnSe indicates the indecisive role of the orthorhombic structure in achieving low for SnSe and provides fresh insight in understanding the thermal properties of SnSe. Furthermore, the even lower of the rock salt SnSe we have identified establishes a possibility for even larger zT materials compared with the orthorhombic SnSe.

We believe that the present work is important and timely hence will be of great interest to the readers of computational materials science.

Thank you for your consideration.

Sincerely,

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