Thermoelectric Materials Modelling

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Recent developments in hardware and software computer technologies together with the development of accurate materials modeling techniques enable researchers to accurately model various phenomena observed in materials, prediction of their behavior under different conditions and the development/ design of cost-effective materials with improved or desired properties. Nowadays, it is possible to perform such simulations even for a large number of materials using the advantages of new neural network and big-data algorithms.

Efficient thermoelectric materials research, as a topical materials science and condensed matter physics problem, has been a good candidate to be investigated with state-of-the-art materials simulation techniques due to the complexity of the experimental procedure and large number of possible candidate materials. Highly accurate predictions, in particular regarding the effect of defects, grain boundaries, and dimension reduction on both electronic and thermal transport properties have led to discovery of novel thermoelectric materials and new directions to experimental studies on already known thermoelectric materials.

Within the past 10 years, we also have investigated thermoelectric properties of both bulk and nano materials by means of density functional theory and molecular dynamics simulations. Our systematic studies on the in particular controlling the thermal transport properties of the novel nano materials, in order to enhance thermoelectric figure of merit of the materials, have been also one of the pioneering studies in the literature and inspired many new studies. The model interatomic potentials developed within the scope of our TE research effort have been still extensively used in the literature.