5th International Symposium on
Energy Challenges & Mechanics
- working on small scales

10-14 July 2016
Inverness, Scotland, UK

Theory and simulation for improving thermoelectric performance of nanoscale materials

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Accepted for publication on 19th February 2016

Thermoelectric materials have undergone revolutionary progress over the last 20 years. The thermoelectric figure of merit ZT, which quantifies the ability of a material to convert heat into electricity has more than doubled compared to traditional values of ZT~1, reaching values even beyond ZT~2 in some instances. These improvements are mostly attributed to drastic reductions of the thermal conductivity in nanostructured materials. However, as thermal conductivities in these structures approach the amorphous limit, any further benefits to ZT must be achieved through the improvement of the thermoelectric power factor. In this work I present theoretical and simulation approaches to compute the thermoelectric power factor in Silicon-based semiconductor nanomaterials. I describe the computational techniques that utilize channel description from continuum to atomistic, and electronic transport from semiclassical to fully quantum mechanical. I focus on two main geometries of nanomaterials, namely low-dimensional materials and nanostructured materials. In the first category, I explain how the electronic bandstructure of a material can be engineered using quantum confinement techniques to improve the electronic conductivity and the thermoelectric power factor. In the second category case, I explain how a material can be engineered to achieve very large power factors, as recently we have demonstrated experimentally as well. In particular, a combination of: i) modulation doping, ii) electron energy filtering through the use of potential barriers, iii) the use of high energy carriers, and iv) two use of more than one material phases, can provide at least a five-fold improvement in the thermoelectric power factor of the material. Such power factor improvement, together with the drastic reduction of the thermal conductivity in nanomaterials, opens a new direction in thermoelectric materials research that could allow unprecedentedly high conversion efficiencies.

Keywords: thermoelectricity, theory and simulation, power factor, energy conversion