Looking for graphene like material for thermoelectric applications

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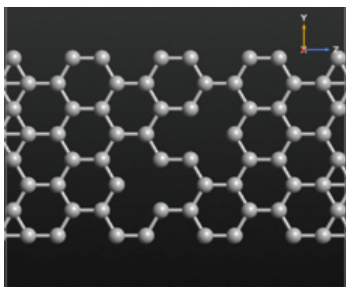
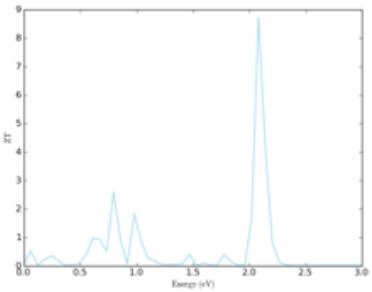
The recent advances in the fabrication and characterization methods of graphene have enable potential applications of graphene in many fields, such as nanoelectronics or thermal management. For the latter, the investigation of heat (phonon) transport is of particular interest [1]. The figure of merit for thermoelectric application *ZT* is proportional to the electric conductivity and inversely proportional to the thermal conductivity of a material. Therefore, it is very desirable to modify a material in such a way that the thermal conductivity reaches the lowest possible value and the electric conductivity retains the value similar to the pristine material. Since the graphene has very high electric conductivity, there is huge space for modifications that could diminish thermal conductivity.

In this report we describe results of extensive modeling performed with Atomistix ToolKit numerical package [2] for various kinds of modified graphene, silicene, and h-BN. This tool allows for direct calculation of the figure of merit *ZT*. We have modeled following modifications of the considered layered materials: (i) bending of nano-ribbons according to a prescribed pattern, (ii) creating in the layer various concentration of simple vacancies, (iii) creating in layers so-called 5-7 defects, (iv) lateral superlattices (graphene/BN, Si/Ge), (v) various decoration of layers with various concentration of atoms C, B Si, Ge, (vi) functionalization of layers with simple molecules.

The results of the modeling can be summarized as follows. The best effect on thermoelectric parameters is observed in structures with vacancies. In the case of h-BN the tremendous increase of *ZT* has been observed for low energies, which is a very desirable effect. In contrary to vacancies, the 5-7 defects have very negative influence on the thermoelectric parameters. Some improvement of the thermoelectric parameters can be also observed in graphene functionalized with C_5H_5N molecule. Exemplary defected graphene layer and calculated *ZT* figure of merit are depicted below.





[1] S. Sadeghi, M. T. Pettes, and Li Shi, “Thermal transport in graphene”, *Solid State Communications* **152**, 1321 (2012).
[2] quantumwise.com