Thermoelectric properties of two- and one-dimensional silicene and germanene from first-principle calculations

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Abstract:

It has been shown recently that the figure-of-merit of graphene nanoribbons embedded by hexagonal boron nitride can be remarkably enhanced [1]. Based on density-functional theory here we investigate the thermoelectric energy conversion efficiency of atomically thin Si and Ge, i.e., silicene and germanene [2]. We consider both the two-dimensional silicene and germanene, together with nanoribbons of different widths. For the nanoribbons, we have also investigated the possibility of nanostructuring these systems by mixing Si and Ge. We found that the figure of merit at room temperature of these systems is remarkably high, up to 2.5.

[1] K. Yang, Y. Chen, R. D'Agosta, Y. Xie, J. Zhong, and A. Rubio, Phys. Rev. B **86**, 045425 (2012).
[2] K. Yang, S. Cahangirov, A. Cantarero, A. Rubio, R. D'Agosta, Phys. Rev. B **89**, 125403 (2014).