Thermoelectric properties of two-dimensional materials: *ab initio* study

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Owing to the possibility of fairly easy tuning of their properties through the suitable structural modifications, 2D layered materials (e.g., graphene, silicene, germanene, transition metal dichalcogenides, MXenes) have emerged recently as very promising candidates for novel devices in the fields of opto- and electronics, spintronics, quantum computing, and recently also for thermoelectric applications. The figure of merit for thermoelectric devices (*ZT*) favors systems characterized by (i) large Seebeck coefficient and (ii) by the as large as possible ratio of electric to the thermal conductivity. Therefore, it has been proposed to introduce structural defects to these materials or perform suitable functionalization of them just to diminish their thermal conductivity. On the other hand, it is fairly well known that alloying can also reduce the thermal conductivity and can be important for thermoelectrics.

In this communication, we present results of extensive studies of thermoelectric properties of pristine and defected monolayers of graphene, silicene, germanene, hexagonal SiGe alloys, and transition metal carbides and nitrides (called MXenes). MXenes joined recently the family of atomically thick 2D layered materials, and preliminary studies indicate that they can outperform 'traditional' 2D materials in many fields. Here, we study thermoelectric properties of some typical representatives of the MXenes group, namely TM_2X, with TM = Ti, and V, and X = C or N, forming tri-layer with layer of material X sandwiched between two layers of transition metals. In the present studies we consider also the transition metal layers being alloys of Ti and V. We consider stripes of these materials of nanometer length and consider the thermoelectric properties in regime of coherent quantum electronic transport. Our studies employ *ab initio* calculations in the framework of the density functional theory for structural and electronic static properties of the investigated systems and non-equilibrium Green's function (NEGF) approach to describe the electronic transport. The major part of the calculations has been performed employing computer packages *TransSIESTA*, *AtomistixToolkit*, and *VASP*.

Our studies reveal that SiGe nanoribbons have generally much better thermoelectric characteristics than graphene, silicene and germacene. The figure of merit *ZT* for SiGe ribbons reaches very promising values, exceeding the required for reasonable thermoelectric systems *ZT* of two, already in very slightly defected SiGe layer. A considerably smaller value of *ZT* for graphene can be achieved only through extremely sophisticated functionalization. The preliminary results for studied MXenes structures with alloyed TM layers and simple structural defects (vacancies) give the value of *ZT* larger than two, indicating that figure of merit can be further increased through suitable engineering of the morphology of the thermoelectric elements based on MXenes. Presently, intensive modeling to find the optimal structures is under way.

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