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Effects of random vacancies on the spin-dependent thermoelectric properties of silicene nanoribbon

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In thermal devices, the capacity to transform heat into electricity and viceversa is characterized by the thermoelectric efficiency, which is usually described in term of the dimensionless quantity $ZT = S^2\sigma T/\kappa$ called figure of merit [1]. In this definition, S is the Seebeck coefficient, σ is the electronic conductance and κ is the thermal conductance at a temperature T, respectively [2]. It is well known that in a thermoelectric system, both electrons and phonons contribute to heat current, then, the thermal conductance can be written as $\kappa = \kappa_{\mathrm{el}} + \kappa_{\mathrm{ph}}$ when electron-phonon coupling is weak. In order to obtain an enhanced thermoelectric efficiency, it is necessary simultaneously reduce both contributions to the thermal conductance without affecting electronic conduction [3]. This can not be obtained in bulk metallic materials due to the classical Wiedemann-Franz law, which establishes that the ratio $\sigma T/\kappa_{\mathrm{el}}$ is a universal constant. Thus, several possible routes to improve the thermoelectric materials have been proposed, such as: i) a controlled reduction of the lattice thermal conductance κ_{ph} by increasing phonon scattering (for instance by nanopatterning with either antidots, defects, or edge modification), ii) enhancing the electron-hole asymmetry at the Fermi energy (by edge roughness or by ferromagnetic insulator substrates in proximity to the system) and iii) the effects of diluted disorder potentials, produced by imputiries, point defects or vacancies, among others [4].

In this work we investigate the spin-dependent thermoelectrical properties of silicene nanoribbons heterostructure, composed by a central conductor with a random distribution of vacancies, connected to two pristine leads of the same material, placed over ferromagnetic insulators. We have considered two configurations for the leads, with the magnetic moments of the left and right lead being parallel or antiparallel. Besides, there is a temperature difference between the leads, giving rise to thermoelectric effects. By using a tight binding Hamiltonian and within the Green´s function formalism and the linear approximation, we have calculated the charge and spin-dependent Seebeck coefficient, the thermal conductance (phonon and spin resolved electronic contribution) and the charge and spin figure of merit of the system, as a function of the geometrical confinement and the concentration of vacancies. Our results exhibit an enhancement of the charge and spin dependent thermopower and the consequent improvement of the thermoelectrical efficiency at room temperature, suggesting that defected silicene nanorribons can be efficient for thermoelectric devices.

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