Thermoelectricity in Non-Periodically Segmented and Branched Nanowires: A Real-Space Renormalization Approach
JOSE EDUARDO GONZALEZ, VICENTA SANCHEZ, CHUMIN WANG, Universidad Nacional Autonoma de Mexico — The direct conversion between thermal and electrical energies by thermoelectric low-dimensional devices has become an important alternative, whose efficiency is determined by the dimensionless figure-of-merit defined as $ZT = \sigma S^2 T / (\kappa_{el} + \kappa_{ph})$, where the Seebeck coefficient ($S$), electrical conductivity ($\sigma$), electronic ($\kappa_{el}$) and phononic ($\kappa_{ph}$) thermal conductivities have an inherent correlation making difficult to improve $ZT$. In this work, we study thermoelectric properties of periodic and quasiperiodically segmented and branched nanowires by means of a real-space renormalization plus convolution method [1] developed for the Kubo-Greenwood formula, in which tight-binding and Born models are respectively used for the calculation of electric and lattice thermal conductivities. This method has the advantage of being computationally efficient, without introducing additional approximations, and capable to analyze aperiodic nanowires with truly macroscopic length. Analytical results are found for periodic nanowires showing a maximum $ZT$ in the temperature space, as occurred in the carrier concentration one. Moreover, the quasiperiodicity seems to be an important $ZT$ enhancing factor [2], since it significantly diminishes the thermal conduction at low temperature of long wavelength acoustic phonons which do not feel local defects neither impurities. [1] V. Sanchez and C. Wang, Phys. Rev. B 70, 144207 (2004). [2] J. E. Gonzalez, V. Sanchez, and C. Wang, J. Electron. Mater. (2017) doi: 10.1007/s11664-016-4946-y

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