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ABSTRACT:

Energy filtering of slow electrons by selective scattering or potential barriers allows for ultra-high thermoelectric power factors in metals and semimetals

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A thermoelectric (TE) generator is a solid-state device which directly converts heat-flux in electricity, and vice-versa. Its efficiency is related to the performance of the TE material, quantified by the figure of merit ZT = σS2T/(κe+κL), where σ is the electrical conductivity, S is the Seebeck coefficient, T is the absolute temperature, and κe and κL are the electronic and lattice parts of the thermal conductivity, respectively. The product σS2 is called the power factor (PF). While ZT improvement targeted mostly thermal conductivity reductions by nanostructuring, the PF is recently tackled with engineered potential barriers in nanostructures, capable of filtering low energy carriers, [1] and with the complex features that new materials exhibit in their electronic structure. [2]
Here, using theory and simulations, we unveil that in metals with overlapping asymmetric bands, band asymmetry (combining very light and very heavy bands) can also allow for very high PFs. The necessary condition other than high asymmetry is strong inter-band scattering, which leads to strong scattering of the low energy carriers of the light band by the heavy band, essentially leading to filtering of low energy charge carriers via selective scattering. We show that PFs of even up to an order of magnitude compared to those of typical semiconductors can be achieved. We establish that the fundamental ingredients are represented by bands overlap, asymmetry, and inter-band scattering. Such effects can be observed in alloys between transition metals with light s- and heavy d-bands, as recently demonstrated for AuNi alloys [3], or of Heusler alloys with an overlap between conduction and valence bands. This new conceptual direction challenges the notion of low TE performance in metals and paves the way to a concrete new research path.

[1] N. Neophytou, et al., Eur. Phys. J. B, 93, 213 (2020), colloquium.
[2] P. Graziosi, N. Neophytou, ACS Appl. Electron. Mater., 10.1021/acsaelm.3c00887, (2023).
[3] F. Garmroudi et al., Sci. Adv. 9, eadj1611 (2023).