Thermoelectric Properties of 2D Materials exhibiting a Mexican-Hat band Structure: An Analytical and Computational Investigation

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The electronic band structures of two-dimensional (2D) materials often exhibit non-parabolic and highly anisotropic features near the valence-band edge. A particularly interesting case is the Mexican-hat-like dispersion, which is characterized by a ring-shaped energy extremum in momentum space. This specific topology leads to a van Hove singularity in the 2D density of states (DOS) and a sharp onset in the electronic transmission spectrum, which can significantly enhance thermoelectric performance. However, real materials often exhibit angular anisotropy in these dispersions, which can shift the DOS singularity and reduce transport efficiency. This study explores the interaction between anisotropy in Mexican-hat-like band structures and thermoelectric properties across a range of 2D materials(1).

Using first-principles density functional theory (DFT) and density functional perturbation theory (DFPT), we systematically investigate seven monolayer compounds: PbBrF, PbClF, PbIF, BaHI, BiOCl, CaHBr, and SrHI. We performed structural optimization, analyzed the electronic band structure, and conducted phonon calculations for each material. Subsequently, we calculated the thermoelectric transport coefficients using the semi-classical Boltzmann transport equation. We then evaluated the phonon-limited lattice thermal conductivity by first determining the third-order force constants and using these with the ShengBTE code. Finally, we discussed the thermoelectric performance of these materials by critically comparing the analytical model with our computational data.

References

[1] HILAL, M, & GÜLSEREN, O (2025). Implications of Mexican hat-like band structure on thermoelectric properties. Turkish Journal of Physics 49 (4): 159-168. https://doi.org/10.55730/1300-0101.2782 .

Figures

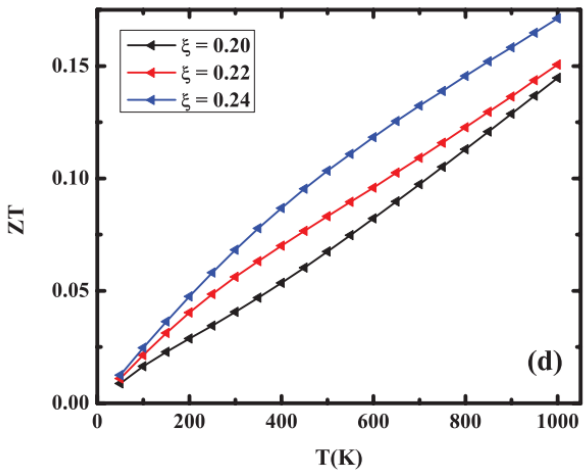

Figure 1: Temperature-dependent figure of merit ZT at μ = 0, showing enhanced thermoelectric performance with increasing ξ .