Anisotropy in phonon and electron transport in Sb_2Se_3 from machine learning foundation models

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The comprehensive evaluation of phonon and electron transport has long been hindered by the fundamental trade-off between *ab initio* accuracy and computational efficiency. The success of machine learning foundation models in mapping potential energy surfaces and electronic Hamiltonian raised the question: can they be extended to predict complex transport properties with high efficiency without sacrificing ab initio accuracy? To answer this question, in this work, we develop a computational workflow integrating state-of-the-art machine learning interatomic potential MACE-MH-1 [1] and Hamiltonian foundation models Uni-HamGNN [2] to investigate the electron and phonon transport properties in Sb_2Se_3. Our results reveal both significant phonon and electron transport anisotropy in Sb_2Se_3: the lattice thermal conductivity exhibits a ~4.8-fold anisotropy, reaching ~2.16 W/mK along the ribbon axis (*x*-axis) and dropping to ~0.66 (*y*-axis) and ~ 0.45 W/mK (*z*-axis) across layers. The pronounced anisotropy in phonon transport originates from the spatial distribution of lone-pair electrons. More specifically, the lone-pair electrons are predominantly distributed within the *yz*-plane, which induces highly asymmetric interatomic forces. This large force asymmetry triggers the highest anharmonic phonon scattering rates, ultimately leading to the ultralow thermal conductivity along the *z*-direction. Furthermore, the carrier mobilities also exhibit remarkable anisotropy. The electron mobility demonstrates a staggering ~48.0-fold contrast between the *x* and *z* directions, while the hole mobility shows a ~5.1-fold variation between the *y* and *z* axes. These electronic anisotropies are primarily driven by significant directional variations in electron-phonon coupling strength and carrier effective mass. This work successfully demonstrates the capability of foundation models to predict complex transport properties with *ab initio* accuracy and remarkable efficiency in Sb_2Se_3.

References

[1] Batatia et al, https://arxiv.org/pdf/2510.25380
[2] Zhong *et al*, Nature Machine Intelligence, 8, 403–414 (2026)

Figure and Table

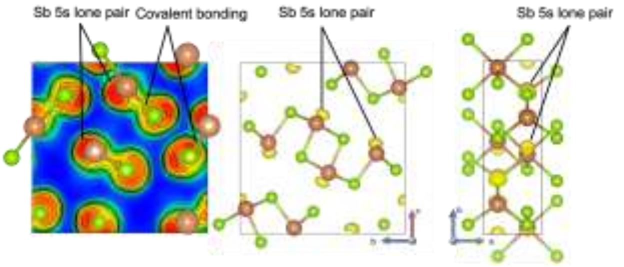

Figure 1. Crystal structure and electronic localization function (ELF) of Sb_2Se_3. Left: ELF plot showing the distribution of Sb 5s lone pairs and covalent bonding regions. Middle and Right: 3D ELF plot of the lone-pair electron density (yellow) relative to the Sb (brown) and Se (green) atomic framework.

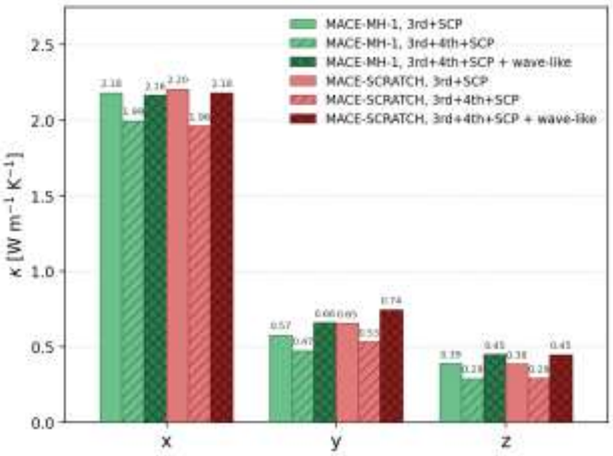

Figure 2. Calculated lattice thermal conductivity along different crystallographic axes. The bar chart compares values calculated using MACE-MH-1 and MACE-SCRATCH models across various levels of theory (3rd order, 4th order, SCP, and wave-like corrections).

Table 1. Directional carrier mobilities and effective masses m* for electrons and holes, where polar denotes the contribution from polar optical phonon scattering and rmp'represents the remaining scattering mechanisms.

$cm^2V^{-1}s^{-1}$	dir	polar	rmp	total	$m^*(m_0)$
Electron	x	99.64	407.24	79.24	0.15
	y	17.92	75.99	14.30	0.89
	Z	2.03	9.65	1.65	7.92
Hole	x	10.94	52.02	8.98	0.97
	y	19.50	97.30	16.13	0.56
	z	3.79	20.33	3.17	2.53