High-throughput calculations of spin Hall conductivity in 2D materials

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Abstract
Maximally localized Wannier functions [1] are widely used to study the electronic and spintronic transport properties. Using the MC2D database [2] and AiiDA manager [3], a Wannierization workflow was developed for the exfoliable 2D materials. From the entire database, all the rare-earth free materials with up to 6 atoms per unit cell were considered, leading to 428 monolayers which were wannierized considering spin-orbital coupling. With this 2D dataset, the room-temperature spin Hall conductivities (SHCs) were calculated using the Kubo formula in the electron- and hole-doped semiconductors and in metals. Figure 1 illustrates our SHC results as a function of crystal structures. The largest SHC can reach up to 5 ($\hbar$/2e)e^2/h in the metallic monolayer. Among all the materials, semimetals are suggested to be promising candidates for efficient charge-to-spin conversion, attributed to the SHC peak at the Fermi energy and the strong scattering in charge transport. Importantly, we find promising novel candidates with exotic spin-orbitronic behaviors with potential applications in electronic devices.

References

[1] Marzari *et al., Rev. Mod. Phys.* **84**, (2012) 1419
[2] Campi *et al., ACS Nano* **17**, (2023) 11268−11278.
[3] Huber *et al.*, *Scientific data* **7**, (2020) 300.

Figures

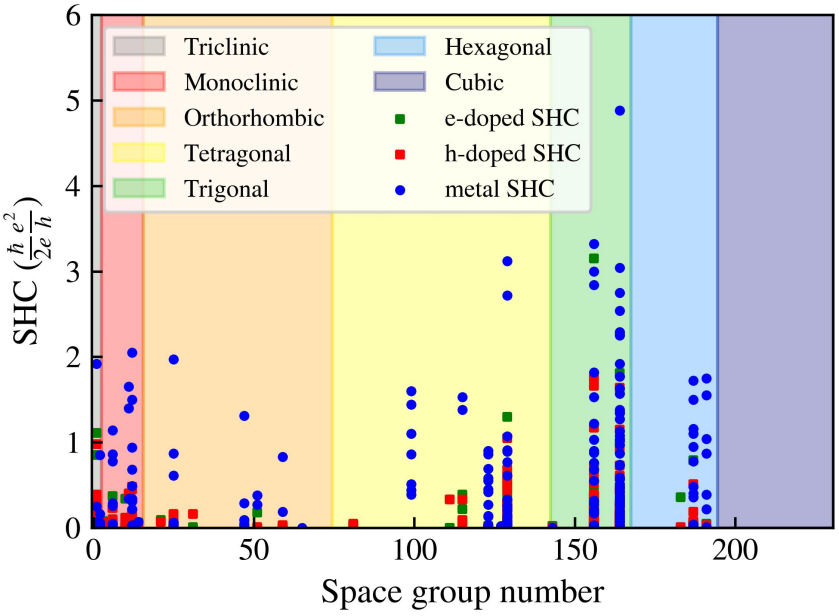

Figure 1: Statistical results of 218 semiconductors doped by electron or hole of 2×10^{13} cm^{-2} concentration, and 210 pristine metals. The horizontal axis denotes the space group numbers of materials, the shaded regions show the structural phases, and the vertical axis indicates the SHC values.