INORGANIC CHEMISTRY SEMINAR

"Thermoelectric transport and crystal chemistry of Zintl Thermoelectrics"

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219 BRL

Zintl phases are salt-like semiconductors with a vast range of structural patterns characterized by covalently-bonded polyanions and electropositive cations. Interest in Zintl phases is motivated by their excellent performance as thermoelectrics materials, which can be used in the conversion of waste heat into electricity. This talk will focus on our recent investigations of chemical bonding anisotropy in Zintl compounds and its impact on their electronic and thermal properties. The first case study is the $Ca_5M_2Sb_6$ (M = Al, Ga, In) system, which form anionic sub-structures resembling infinite 1D chains of corner-linked MSb_4 tetrahedra, leading to predicted quasi-1D electrical conductivity. We were able to confirm this experimentally by growing $Ca_5M_2Sb_6$ single crystals from an Sb-rich molten flux and measuring the resistivity parallel and perpendicular to the growth direction. Surprisingly, despite anisotropic electronic transport, $Ca_5M_2Sb_6$ compounds are predicted to have isotropic thermal transport, thanks to the strong ionic bonds between Ca and the polyanions. However, not all Zintl compounds exhibit stiff ionic bonds. Indeed, by tuning the cation bonding environment, we can induce soft vibrational modes that are beneficial for thermoelectric applications, as demonstrated in the AMg_2Sb_2 (A = Mg, Ca, Yb) series. Here, we use a combination of resonant ultrasound spectroscopy, inelastic x-ray scattering, and high-pressure diffraction to study the effect of the cation size on local bonding, and its impact on thermal conductivity. We find that if the cation is too small for the octahedral site, the result is a softening of the shear vibrations, leading to anomalously low lattice thermal conductivity when A = Mg.

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