Seminar/Talk

Antibonding Electronic States: Not Always a Devil

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Host: Maria Ibáñez

Fundamental understanding of the nature of chemical bonding and its influence on the electronic structure is paramount to chemistry, solid state physics and materials science. CuBiI4 has a fascinating structure where Cu and Bi are surrounded by a tetrahedral and octahedral halogen framework respectively. From fundamental inorganic chemistry concepts, it is expected to have symmetry-allowed d-p overlap in the tetrahedral co-ordination and we see here strong Cu (d)- I (p) strong interaction. This rare interaction generates an antibonding state in the valence band just below the Fermi energy in the electronic structure. Electrons filling up the antibonding band weaken the bond and subsequently the crystal lattice becomes soft and anharmonic giving rise to ultra-low thermal conductivity. In the latter part of my talk, I will be talking about achieving an ultralow value and unusual glass-like temperature dependence of lattice thermal conductivity in a large single crystal of layered halide perovskite Cs3Bi2I6Cl3. Here, Bi-Cl interaction also forms a s-p antibonding state below the Fermi level which renders a soft lattice. While strong anharmonicity originates from the low energy and localized rattling-like vibration of Cs atoms, synchrotron X-ray pair-distribution function analysis further evidences the presence of local structural distortions in the Bi-halide octahedra. We propose that hierarchical chemical bonding, presence of antibonding states near Fermi level and low energy vibrations from selective sublattice in crystalline inorganic halide perovskites open an intriguing avenue for thermal transport research with their unfathomed lattice dynamics and potential applications.

Friday, September 22, 2023 11:00am - 12:00pm
Office Bldg West / Ground floor / Heinzel Seminar Room

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