INDIAN ASSOCIATION FOR THE CULTIVATION OF SCIENCE

2A & 2B, Raja S. C. Mullick Road, Jadavpur, Kolkata-700 032

School of Materials Science

SEMINAR NOTICE

Title of the Talk: "Chemical Bonding and Structural Design of Quantum Materials for Thermoelectrics"

Speaker: Kaniska Biswas

Date: July 24, 2025 (Thursday)

Time: **16:00 hours (IST)**

Venue: C V Raman Hal

Abstract: New Chemistry Unit, International Centre for Materials Science and School of Advanced Materials, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR),
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Chemical bonding is a chemist's most fundamental tool to control and optimize material properties - especially crucial when addressing the competing demands of electrical and thermal transport in thermoelectrics. In topological quantum materials, where unconventional electronic states coexist with complex lattice dynamics, bonding design plays a pivotal role. Recently, metavalent bonding has attracted attention for balancing covalent localization and metallic delocalization of electron, offering a path to overcome the phonon–electron trade-offs that limit thermoelectric performance.

Meanwhile, the concept of a homologous series, rooted in mathematics as a systematically ordered sequence, has gained renewed importance in solid state chemistry as a guide for new structure prediction. Phase homology refers to a family of structures constructed on a common architectural principle, where specific structural units expand along one or more dimensions in a regular, modular fashion. Stabilizing such homologous series in crystalline solids enables controlled repetition of motifs, offering a rational strategy to tune bonding interactions, modulate lattice vibrations, and

systematically engineer topological electronic states.

This talk presents a chemical design framework that integrates metavalent bonding, lone pair chemistry, and homologous series engineering to suppress heat transport while enhancing electronic performance in certain quantum materials. We begin with a 3D topological insulator like TlBiSe2, where the cooperative action of dual lone pairs and metavalent bonding induces local structural distortions and lattice shearing, effectively

damping phonons.1 Extending this approach, we explore BiSe, a weak topological insulator from the (Bi2)m(Bi2Se3)n series, where insertion of Bi2 bilayers introduces soft vibrational modes that strongly couple with heat-carrying acoustic phonons reducing lattice thermal conductivity.2 Similar design logic has been applied to BiTe, a dual topological insulator, where pressure-enhanced metavalent bonding drive electronic topological transitions and alter phonon behavior.3 Finally, we examine Sb-based layered homologues, (Sb2)m(Sb2Te3)n where structural modulation through Sb2 bilayer insertion enables shear-softened lattices that resist thermal transport.4

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Samanta, M.; Pal, K.; Pal, P.; Waghmare, U. V.; Biswas, K. J. Am. Chem. Soc., 2018, 140, 5866.
Pathak, R.; Joseph, A.; Dutta, P.; Joseph, B.; Duhan, J.; Chandra, S.; Narayana, C.; Pal, K.; Biswas, K. Angew. Chem. Int. Ed., 2025, 64, e202422652.
Das, S.; Biswas, S.; Francis, A. G.; Acharyya, P.; Biswas, R. K.; Das, A.; Ghatak, J.; Pati, S. K.; Biswas, K. Adv. Energy Mater., 2025, 2500688.

All are cordially invited to attend the Seminar.