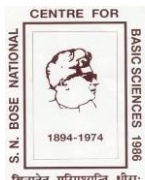


INSTITUTE COLLOQUIUM



विज्ञानेन परिपश्यन्ति धीराः



5th June 2023
4.00 pm at
FERMION Hall

TITLE: Metavalent chemical bond holds key to enhance the thermoelectric performance in quantum materials

ABSTRACT: Chemical bonding is a chemist's strongest tool to tailor and tune material properties, especially when optimizing material attributes like the thermoelectric performance that is composed of conflicting correlations between electrician thermal transport in crystalline solids. Metavalent bonding has recently attracted immense attention owing to its capability to impart distinct property portfolio in crystalline solids. It is an exemplary and distinct bonding, characterized by the fine tuning between the localization (covalency) and delocalization (metallicity) of the bonding electrons. Thus, the unique features of metavalent bonding can directly address the thermoelectric challenge.

While searching for materials with excellent electrical properties, our attention was drawn by quantum materials such as topological insulators. They are an exotic family of compounds that have metallic surface states but semiconducting bulk states. Due to their special electronic band structure, they show high carrier mobility harbouring intriguing electrical transport. This class of materials share many design features with thermoelectric materials, like having heavy atoms, low band gap, spin-orbit coupling etc. Due to the shared chemical design pool, topological materials are also potential thermoelectric materials and many of them show metavalent bonding.

A change of bonding type from covalent to metavalent was realized in GeSe by alloying it with AgBiTe.^[2] Our strategy increased the zT from ~ 0.2 in pristine GeSe to ~ 1.35 in $(\text{GeSe})_{0.9}(\text{AgBiTe}_2)_{0.1}$ at 627 K.^[1] Further, guided by the unique properties offered by metavalent bonding and lone pair expression, our recent work on quantum materials, TlBiSe ^[2] demonstrated that employing metavalent bonding could be an elegant way to devise a configurational under-constraint in crystalline solids to allow degenerate manifold of ground states that can be easily accessed through slight structural distortions induced by lone pair expression. The soft p-bonding network in TlBiSe ^[2] facilitates long-range propagation of the dual lone-pair induced lattice anharmonicity, revealing a new channel to intrinsically lower thermal conductivity.^[2]

1. Sarkar, D.; Roychowdhury, S.; Arora, R.; Ghosh, T.; Vasdev, A.; Joseph, B.; Sheet, G.; Waghmare, U. V.; Biswas, K. *Angew. Chem. Int. Ed.* 2021, 60, 10350-10358.
2. Maria, I.; Arora, R.; Dutta, M.; Roychowdhury, S.; Waghmare, U. V.; Biswas, K. *J. Am. Chem. Soc.* 2023, 145, 9292-9303.



SPEAKER: Prof. Kanishka Biswas is a Professor at the New Chemistry Unit (NCU) & School of Advanced Materials (SAMat) at Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR). Prof. Biswas obtained his MS and Ph.D. (2009) degree from the Indian Institute of Science (IISc) and subsequently did his postdoctoral research (2009–2012) at Northwestern University before joining JNCASR in 2012.

He is a recipient of S.S. Bhatnagar Award (2021) and is a fellow of the Indian Academy of Sciences. His research area includes Solid State Chemistry of Metal Chalcogenides /Chalcohalides, Thermoelectric Materials, 2D layered materials, Topological insulators, Halide Based Perovskites, Water Purification etc.

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