Institute Colloquium

S. N. Bose National Centre for Basic Sciences
(An Autonomous Research Institute established under DST, GOI)

24 April, 2023 | **4 PM at FERMION, SNBNCBS** | **Webinar Link** | **YouTube Link**

Title:

Layered Hybrid Perovskites: Molecular Design and Optoelectronics

Abstract:

Hybrid perovskites like $(C_4H_9NH_3)_2PbI_4$ have fascinating layered crystal structure with periodic nanoscale interfaces between the inorganic $\{PbI_4\}^{2-}$ and organic $C_4H_9NH_3^+$ layers. Because of these interfaces, electron and hole are confined in atomically thin $\{PbI_4\}^{2-}$ inorganic well layers. Therefore, these layered perovskites are electronically 2D systems (quantum well), irrespective of their crystallite sizes.[1,2] Importantly, the crystal structure allows numerous combinations of different organic cations and inorganic anions. So a rational molecular design of the nanoscale interfaces, and hence, tunable optoelectronic properties are feasible. For example, if structural non-centrosymmetry is introduced in such semiconductors, then important functionalities like chirality, non-linear optical properties, ferroelectrocity, and anomalous photovoltaic effect can be achieved. In this talk, I will discuss about design principles of achiral and chiral non-centrosymmetric hybrid perovskite single crystals. The key parameter that yields the desired non-centrosymmetric structure is the rationally designed non-covalent (hydrogen- and halogen-bonding) interactions, between the organic cation sublattice and the inorganic $\{PbI_4\}^{2-}$ sublattice.[3] Furthermore, I will also discuss about how non-covalent cation-pi interactions between the A-site cations can make low-dimensional hybrid metal halides completely water-stable for years.[4-5]

References:

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3. Chakraborty, R.; Rajput, P. K.; Anilkumar, G. M.; Maqbool, S.; Das, R.; Rahman, A.; Mandal, P.; Nag, A. J. Am. Chem. Soc.**2023**, 145, 1378 −1388.
4. Sheikh, T.; Maqbool,S.; Mandal, P.;Nag, A.Angew. Chem. Int. Ed.**2021**,60,18265 −18271.
5. Sheikh, T.; Anilkumar, G. M.; Das, T.; Rahman, A.;Chakraborty, S.; Nag, A. J. Phys. Chem. Lett.**2023**, 1870−1876.

Speaker:

Dr. Angshuman Nag

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Short biography of the Speaker

Dr. Angshuman Nag completed his Master of Science in Chemistry from IIT Guwahati in 2003, and obtained his PhD from IISc Bangalore in 2009. He then completed two terms as postdoctoral researcher at IISc Bangalore and at the University of Chicago. In 2012, he started his own research group at IISER Pune as a Ramanujan Fellow. Presently, he is an Associate Professor.