

INDIAN ASSOCIATION FOR THE CULTIVATION OF SCIENCE

2A & 2B, Raja S.C. Mullick Road, Jadavpur, Kolkata-700032,

India

Seminar Notice

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School of Physical Sciences

Title:	Unique Super-Ionicity Achieved on the Nanoscale with Applications in Energy-Relevant Materials
Speaker:	Dr. Proгна Banerjee, University of Illinois at Urbana-Champaign, USA.
Date:	December 10, 2018 (Monday)
Time:	3:30 p.m.
Venue:	Physics Seminar Room - C404, 3rd Floor, Centenary Building, IACS
Abstract:	I employ a topotactic method called cation exchange to produce semiconductor nanocrystals (NCs) in novel morphologies, compositions, and crystallographic phases. My dissertation research focuses on the understanding of the physical properties and phase transitions of these new nanomaterials prepared by cation exchange¹⁻³. In this talk, I shall describe the countless possibilities of the exploration of physicochemical properties and applications of molecularly precise semiconductor nanoclusters, a class of materials that we were able to expand with the help of cation exchange. In particular, I shall discuss how ultrasmall copper selenide (Cu_{2-x}Se) NCs prepared by cation exchange of cadmium selenide NCs exhibit a disordered cationic sub-lattice under ambient conditions¹. Known superionic materials, such as AgI, Cu_2Se etc. in their bulk form, display this phase transition at high temperatures and/or pressures, making them unsuitable for many applications. As a follow-up to this study, I shall describe my investigations of Li-doping of Cu_{2-x}Se NCs and how this doping influences the crystal structure and consequently the phase transition behavior². We are extending this work to investigate the possible mechanism of ionic transport in these NCs using AC impedance measurements. We are investigating size and dimensionality effects on the transport behavior of cations and the superionic phase transition. We will also

investigate the effect of cation vacancies in terms of their profile and density on the phase transition behavior and ionic conductance. This study will pave the way to fundamental understanding on ion transport behavior in solids, and applications as solid-state electrolytes, thermoelectric and ultrafast electronic switches. If time permits, I shall explain on the basis of optical spectra measurements and density functional theory (DFT) calculations how HgSe NCs³, prepared using cation exchange is found to have an inverted band structure along with a finite band-gap, making it a potential 3D topological insulator.

References: 1. White[†], S. L., Banerjee[†], P. & Jain, P. K. Liquid-like cationic sub-lattice in copper selenide clusters. *Nat. Commun.* **8**, 14514 (2017). († denotes equal contribution)

2. Banerjee, P. & Jain, P. K. Lithiation of Copper Selenide Nanocrystals. *Angew. Chem. Int. Ed.* **57**, 9315–9319 (2018).

3. Dumett Torres, D., Banerjee, P., Pamidighantam, S. & Jain, P. K. A Non-Natural Wurtzite Polymorph of HgSe: A Potential 3D Topological Insulator. *Chem. Mater.* **29**, 6356–6366 (2017).