S N BOSE NATIONAL CENTRE
FOR BASIC SCIENCES
Block JD, Sector III, Salt Lake, Kolkata 700 106

DEPARTMENTAL SEMINAR

Condensed Matter and Materials Physics

16th January,2024 **4.00 PM** **ONLINE/ FERMION**

SPEAKER

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TITLE OF THE TALK

EFFECTIVE MODEL AND EFFICIENT ALGORITHM :
A TALE OF TWO TOOLS FOR PLASTIC SEMICONDUCTOR DISCOVERY

ABSTRACT

Organic semiconductors are quite fascinating due to their structural flexibility, chemical tunability, ease of processing and low cost while the subtle interplay between their electronic structures and geometric structures results in a rich variety of physical phenomena. These π-conjugated systems promise the advent of fully flexible opto-electronic devices like light emitting diodes, field effect transistors and photovoltaic cells. However, full potential of these plastic semiconducting materials can only be realized with the fundamental understanding of the nature of the electronic excitations and transport phenomena within these materials which are difficult to deduce within conventional quantum chemical approaches. The softness of the structural moieties, coupling between electronic and vibrational degrees of freedom, van der Waals nature of inter-molecular interactions and quasi-one dimensionality of the π-conjugation network, leading to enhanced long-range electron-electron correlation, brings about complexity in the electronic structure and dynamics, and multi-scale computational approaches are most suitable for investigating these semiconducting materials.

In this talk, we will deliberate on the usefulness of effective physical models, in conjunction with advanced numerical techniques in probing essential features of promising π-conjugated materials. We will primarily focus on the modelling of charge(energy)-carrier transport within disordered organic semiconductors and elaborate on the structure-transport property relationships. We will present applications of non-adiabatic molecular dynamics technique to explore intra-chain charge transport mechanism within disordered polymer semiconductors and will demonstrate how a simplified but physically sound model can capture the important effects of both local and nonlocal electron-phonon interactions associated with conformational motion on carrier dynamics. 1,2 We will also briefly discuss the usefulness of this approach in investigating efficient energy transport within polymer nanofiber films. 3 The relevance of a robust model reduction scheme for polymer semiconductors will also be illustrated which can capture the chemical details and can be employed to rapidly compare different polymers or to perform virtual screenings. 4 We will conclude the talk with future outlooks and emerging fields within the realm of organic π-conjugated materials.

References:
1. Prodhan, S. et al. Design Rules to Maximize Charge-Carrier Mobility along Conjugated Polymer Chains. J. Phys. Chem. Lett. 11, 6519–6525 (2020).
2. Dilmurat, R., Prodhan, S., Wang, L. & Beljonne, D. Thermally activated intra-chain charge transport in high charge-carrier mobility copolymers. J. Chem. Phys. 156, 084115 (2022).
3. Sneyd, A. J. et al. Efficient energy transport in an organic semiconductor mediated by transient exciton delocalization. Sci. Adv. 7, eabh4232 (2021).
4. Prodhan, S., Manurung, R. & Troisi, A. From Monomer Sequence to Charge Mobility in Semiconductor Polymers via Model Reduction. Adv. Funct. Mater. 33, 2303234 (2023).

HOST FACULTY

Dr. Nitesh Kumar, Assistant Professor

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