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

# DEPARTMENTAL SEMINAR

## Condensed Matter Physics and Material Sciences

**01st December'2021 4.00PM ONLINE**

### SPEAKER

**Dr. Kapildeb Dolui,**
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**Lomare Technologies, Imperial College London**

### TITLE OF THE TALK

Computational Spintronics in 2D Quantum Materials

### ABSTRACT

The discovery of the giant magnetoresistance effect, celebrated by the 2007 Nobel Prize, has generated a revolutionary impact on the data storage technologies such as magnetoresistive random access memory (MRAM). This triggered the rise of Spintronics, an interdisciplinary field which involves the study of active control and manipulation of spin degrees of freedom in solid-state systems. Spin-orbit-torques (SOTs), which rely on spin current generation from charge current in a nonmagnetic material, promise an energy-efficient scheme for manipulating magnetization in Spintronic devices. A critical topic for spintronic devices using SOTs is to enhance the charge to spin conversion efficiency. In this talk, I will discuss how the different classes of 2D materials, namely transition-metal chalcogenides (CrI3, WSe2, TaSe2 etc.), topological insulators (Bi2Se3), and Weyl semimetals (WTe2, MoTe2), could emerge as viable source of current-driven SOT [1,2,3]. Subsequently, the current-driven magnetization dynamics is studied by combining calculated complex angular dependence of SOT with the Landau-Lifshitz-Gilbert equation for classical dynamics of magnetization. In addition, I will discuss the quintessence of first-principle based spin-transport calculations for these modeling with quantum materials. In particular, I will show our development of computational methodology using noncollinear density functional theory (ncDFT) Hamiltonian combined with charge conserving Floquet-nonequilibrium Green function formalism (Floquet-NEGF) [4] and with density matrix approach [5] to quantify several spintronics phenomena such as spin-torque, spin pumping, and spin memory loss.

References

[1] J. M. Marmolejo-Tejada et al., Nano Lett. 17, 5626 (2017).
[2] K. Dolui et al., Nano Lett. 20, 2020 (2020).
[3] K. Dolui and B. K. Nikolic, Phys. Rev. Materials 4, 104007 (2020) (Editor's suggestion).
[4] K. Dolui, U. Bajpai, and B. K. Nikolic, Phys. Rev. Materials 4, 121201(R) (2020).
[5] K. Dolui and B. K. Nikolic, Phys. Rev. B 96, 220403 (R) (2017).

### HOST FACULTY

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