

MONDAY

COLLOQUIUM

Computational Modelling of Molecules and Materials for Catalytic and Thermoelectric Applications

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2 Nov 2026 (Monday) | 16:00 Hrs (Tea / Coffee 15:45 Hrs) | Venue: TIFRH Auditorium

Current trend in research on molecules and materials majorly encompasses creation, conversion and storage of renewable energy. In this respect, I shall discuss our efforts in computational modelling of a few molecules and materials (i) which show electrochemical water splitting with hydrogen evolution reaction (HER) at anode and oxygen evolution reaction (OER) at the cathode end, (ii) which show bifunctional electrocatalyst with both OER and oxygen reduction reaction (ORR). We have also been working on modelling thermoelectric materials which convert waste heat into electricity using Wigner-Peierls-Boltzmann semiclassical transport equations together with density functional theory calculations. I shall talk on finding thermoelectricity in 9 Bi based half-Heusler compounds $XYBi$ (X: Ti, Zr, Hf; Y: Co, Rh, Ir) and in a phonon-glass-electron-conductor, $AgGeSnSbTe_4$, which was synthesized and studied by an experimental group. If time allows and scheduling permits, I shall discuss our computational efforts in understanding the very low thermal conductivities observed in two systems, $TlAgSe$ and Tl_2AgI_3 , which were synthesized and studied by an experimental group.