MONDAY

# COLLOQUIUM

## Computational Electrodics: Pressing Issues and Recent Approaches

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

Electrodics, a subfield of electrochemistry, encompasses processes related to electrode-electrolyte interaction and is at the heart of research related to energy conversion (e.g., battery, fuel cell) and storage (e.g., supercapacitors). In this presentation, I will discuss the different topics of interest (and concern) when one tries to model these processes in silico. Two main focuses of this talk will be (i) a novel implementation of an electronic structure method that allowed us to demonstrate the significant contribution of the polarization of the water molecules to the overall interfacial dipole moment at gold-water interface (ii) imposition of a constant potential on the electrode of interest within the framework of ab initio molecular dynamics. Here, I will explain two different approaches along with their strengths and weaknesses. As a promising first step to unify these two approaches, will show that the key concept of one method can be applied within the simulation set-up of the other. Finally, I will show preliminary results on corrosion studies from platinum grain boundaries within force field based molecular dynamics.

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