Bose Colloquium

S. N. Bose National Centre for Basic Sciences

(An Autonomous Research Institute established under DST, GOI)

Title:

Unravelling the Working Mechanisms of Ligand-Gated Ion Channel with Atomistic Simulations

Abstract:

Ligand-gated ion channels (LGICs), embedded in the membrane of nerve cells, are key neuroreceptors that mediate fast synaptic transmission. They play crucial roles in a variety of neurological disorders and are target sites for therapeutical drugs.

These receptors are activated when specific ligands bind to them, triggering conformational changes that culminate with the opening (gating) of an ion-conducting channel in the cell membrane.

Despite their significance, the molecular-level details of their activation mechanisms remain only partially understood, due to their complexity and the limited experimental information available.

In recent years, advances in experimental techniques have provided valuable insights into the relationships between structure and function in LGICs. In this talk, I will show how atomistic simulations, in particular molecular dynamics and the enhanced-sampling method metadynamic, are contributing to our understanding of several key aspects of LGIC function, including ligand binding and unbinding, the molecular switches that mediate channel gating, and the impact of mutations on receptor behaviour.

19th November, 2025

4.00 PM

At Silver Jubilee Hall

YouTube Link

Webinar Link

Speaker: ***Prof. Carla Molteni, Professor of Physics, Co-Director BiPAS CDT & Director at King's, Thomas Young Centre for the Theory and Simulation of Materials, Physics Senior Tutor.***

Short Biography of the Speaker:

Carla Molteni is Professor of Physics at King's College London and is a Fellow of the Institute of Physics. She is an expert in atomistic simulations applied to materials and biological systems, and works at the interface of physics with chemistry, materials science and biology. Before joining King's, Carla held an EPSRC Advanced Research Fellowship at the Cavendish Laboratory, University of Cambridge, and a College Research Fellowship at New Hall (now Murray Edwards College). Previously, she was a postdoctoral researcher at the Max Planck Institut fuer Festkoerperforschung in Stuttgart (Germany) and a EU Human Capital & Mobility Postdoctoral Fellow at the Cavendish Laboratory. She obtained her Laurea and PhD in Physics at the University of Milan (Italy).

Carla is co-Director of the London Thomas Young Centre for the Theory and Simulation of Materials and is deputy Director of the multidisciplinary Centre for Doctoral Training BiPAS (Biological Physics Across Scales). She is member of the management board of the JCMaxwell node of CECAM and of the Materials and Molecular Modelling Hub, and is the leader of the working group "Molecules, Macromolecules and Biomolecules" of the Psik European network. She is also member of the research council of the Italian Embassy in London and of the board of directors of AISUK, the Association of Italian Scientists in the UK.