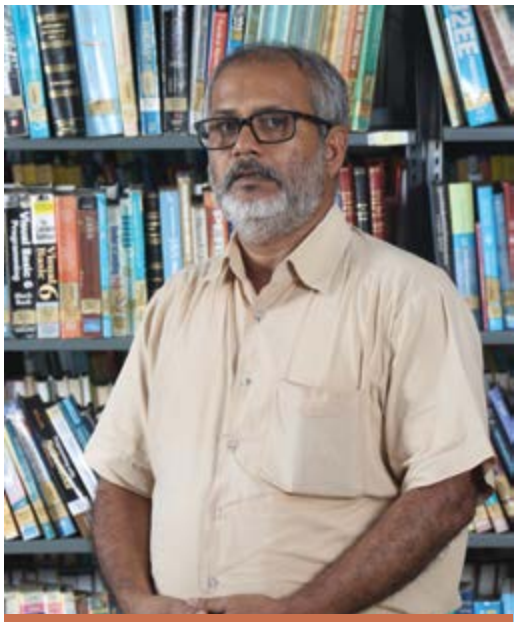

Gautam Gangopadhyay

Professor
CBMS
gautam@bose.res.in

Prof. Gautam Gangopadhyay is working in the broad area of Chemical Physics. It includes statistical mechanical modeling of reaction kinetics for example, in reaction network, ion-channels. They are working on nonlinear dynamical characterization of ion channels and drug binding. They are also interested in quantum nonadiabatic molecular properties theoretically through conduction and spectroscopic tools.

Supervision of Research / Students

Ph.D. Students

1. Krishnendu Pal; Theoretical studies on Sodium ion Channel; Ongoing (to be submitted).
2. Sandip Saha; Nonlinear dynamical studies on Isochronous oscillators in Chemistry and Biology; Ongoing (2015-).

Teaching activities at the Centre

1. Chemical Physics; PHY-404 for Int. PhD students.

Publications in Journals

1. Krishnendu Pal, **Gautam Gangopadhyay;** *Dynamical characterization of inactivation path in voltage-gated Na+ ion channel by non-equilibrium response spectroscopy; Channels;* 2016; **10** (6); 478-497.
2. Krishnendu Pal, Biswajit Das and **Gautam Gangopadhyay;** *Nonequilibrium response of a voltage gated sodium ion channel and biophysical characterization of dynamic hysteresis;* J.Theor. Bio.; 2017; **415;** 113-124.
3. Sandip Saha and **Gautam Gangopadhyay;** *Isochronicity and limit cycle oscillation in chemical systems;* J. Math. Chem.; 2017; **55** (3); 887-910.

Lectures Delivered

1. An Introduction to Nonequilibrium processes at C. K. MAJUMDAR MEMORIAL SUMMER WORKSHOP IN PHYSICS 2016; SNBNCBS; 20.06.2016; One.

Membership of Committees

External Committee

Theoretical Chemistry Symposium-2016, member of National Advisory Committee.

Internal Committee

Member SCRE, EVLP, Patent and Project Cell.

Fellow / Member of Professional Body

1. Life Member of IACS

Conference / Symposia / Workshops / Seminars etc. organized

1. Member National advisory committee; 15th Indian Theoretical Chemistry Symposium; 14-17 December; Hyderabad; Session Chairman.

Significant research output / development during last one year

General research areas and problems worked on

We have done a series of works on sodium and potassium ion channels. This year we have dynamically characterized inactivation path in voltage-gated Na+ ion channel by non-equilibrium response spectroscopy. In the similar context we have estimated the nonequilibrium response of a voltage gated sodium ion channel and biophysical characterization of dynamic hysteresis. In a different context we have found the condition of Isochronicity and limit cycle oscillation in several biochemical system.

Interesting results obtained

Inactivation path of voltage gated sodium ion channel has been studied here under various voltage protocols as it is the main governing factor for the periodic occurrence and shape of the action potential. In contrast to a lot of effort in finding the crystal structure based molecular mechanism of closed-state(CSI) and open-state inactivation(OSI) here our approach is to understand inactivation process through dynamical characterization. The kinetic flux as well as energetic contribution of the closed and open- state inactivation path is compared here for voltage protocols, namely constant, pulsed and oscillating. It is shown that an efficient CSI and OSI dynamical profile in principle can characterize the open-state drug blocking phenomena.

We have introduced a method of estimating the work done associated with the dynamic memory due to a cycle of oscillating voltage. We have quantitatively characterised the loop area of ionic current which gives information about the work done to sustain the dynamic memory only for ion conduction, while the loop area of total entropy production rate gives the estimate of work done for overall gating dynamics. The maximum dynamic memory of Na-channel not only depends on the frequency and amplitude but it also depends sensitively on the mean of the oscillating voltage and here we have shown how the system optimize the dynamic memory itself in the biophysical range of field parameters.

Chemical oscillation is an interesting nonlinear dynamical phenomenon which arises due to complex stability condition of the steady state of a reaction far away from equilibrium which is usually characterised by a periodic attractor or a limit cycle around an interior stationary point. In conjunction with the property of limit cycle oscillation, here we have shown the condition for isochronicity for different chemical oscillators with the help of renormalisation group method.

Proposed research activities for the coming year

1. Role of Patch Size in Synchronization and Metabolic Energy Consumption in Coupled Neurons which is a first step to signal transduction and the effect on synchronization due to Drug Blocking of Sodium and Potassium Channels.
2. Staring from the microscopic study of the Effect of single Sodium And Potassium channels due to drug blocking we have estimated the macroscopic effect on Action Potential.

Any other matter

1. Vigilance Officer of the Centre from Dec'2014.