NATIONAL INSTITUTE OF TECHNOLOGY KARNATAKA Surathkal - 575025

DEPARTMENT OF CHEMISTRY

is organizing Three Days Virtual lecture workshop on " Simulation and modeling in Chemistry"

from 2nd to 4th December 2020 Sponsored by Indian Academy of Science, Bengaluru.

Welcome Remarks : Prof. Arun M. Isloor (HoD Chemistry, NIT K), 11:15 a.m

Presidential Address : Prof. K. Umamaheshwar Rao (Director, NIT K), 11:20 a.m

List of speakers:

(1) Prof. Amalendu Chandra (IIT K)
(2) Prof. E. D. Jemmis (IISc)
(3) Prof. Swapan K. Ghosh (University of Mumbai)
(4) Prof. Swapan Pati (JNCASR)
(5) Prof. Nisanth N. Nair (IIT K)
(6) Dr. Hemant K Kashyap (IIT D)
(7) Dr. Durba Sengupta (NCL, Pune)
(8) Dr. Jagannath Mondal (TIFR H)
(9) Dr. Suman Chakrabarty (SNBNCBS)

Sponsored by:

Indian Academy of Science, Bengaluru, Indian National Science Academy, New Delhi, The National Academy of Science India, Prayagraj

Convenor : Prof. Amalendu Chandra (IIT Kanpur)
Coordinator : Dr. Debashree Chakraborty
(Asst. Professor, NIT K)
Email : debashree@nitk.edu.in

Date/Day	Title of lectures and time schedule			
	11:30am-12:30pm	**2:00pm-3:00pm**	**3:15pm-4:15pm**	**4:30pm-5:30pm**
02-Dec-2020 Wednesday	***Prof. Amalendu Chandra*** Title: **Basic statistical mechanics, molecular simulations and calculations of thermodynamic quantities**	***Dr. Suman Chakrabarty*** Title: **Computational alchemy and acceleration of rare events: some applications to biophysical problems**	***Prof. Swapan K. Ghosh*** Title: **Concept of density and modelling in chemistry across the length scale**	***Dr. Durba Sengupta*** Title: **Coarse-grain approaches in (bio)-molecular simulations: Part 1**
03-Dec-2020 Thursday	**10:00am-11:00am**	**11:15am-12:15pm**	**3:15pm-4:15pm**	**4:30pm-5:30pm**
	Prof. E. D. Jemmis Title: **Qualitative ideas and quantitative simulations**	***Prof. Nisanth N. Nair*** Title: **Free energy landscapes of chemical reactions**	***Dr. Jagannath Mondal*** Title: **Computer simulation of protein ligand binding using coarse grained model**	***Dr. Hemant K Kashyap*** Title: **Stability of thermodynamic phases of modern electrolytes within nanoscale confinement**
04-Dec-2020 Friday	***Prof. Swapan Pati*** Title: **Computational modeling of catalysis: A few examples from heterogeneous and homogeneous catalytic reactions.**	***Prof. Amalendu Chandra*** Title: **Hybrid simulations**	***Dr. Durba Sengupta*** Title: **Coarse-grain approaches in (bio)-molecular simulations: Part 2**	***Dr. Jagannath Mondal*** Title: **Simulating the membrane disruption process by biomimetic peptides**

Day 1 : https://teams.microsoft.com/l/meetup-join/19%3ameeting_YTBlZjgzZGUtYTBmZS00NTExLWI0ZjUtNzk2MmVmMTQxZDUz%40thread.v2/0?context=%7b%22Tid%22%3a%2236e917dc-1abe-43f4-b189-f92196a6b4ad%22%2c%22Oid%22%3a%224fbd32b0-6e2b-4943-91ae-a3213fe61040%22%7d

Day 2 : https://teams.microsoft.com/l/meetup-join/19%3ameeting_MWFjMDUwZDktMjZiNS00ODk0LWI5MGEtYjQ2ZWM1NTZhZTMx%40thread.v2/0?context=%7b%22Tid%22%3a%2236e917dc-1abe-43f4-b189-f92196a6b4ad%22%2c%22Oid%22%3a%224fbd32b0-6e2b-4943-91ae-a3213fe61040%22%7d

Day 3: https://teams.microsoft.com/l/meetup-join/19%3ameeting_YzYzNGZiYTktNzI2Zi00OTA0LTk5YjEtYjU0MmRkNDBlODVk%40thread.v2/0?context=%7b%22Tid%22%3a%2236e917dc-1abe-43f4-b189-f92196a6b4ad%22%2c%22Oid%22%3a%224fbd32b0-6e2b-4943-91ae-a3213fe61040%22%7d