

**03 March 2021, Wednesday**

**09:30 - 09:45 AM**

**Inauguration:**

Session In charge

Sudipta Maiti (Chair, DCS - TIFR Mumbai)

Jagannath Mondal

V. Chandrasekhar (Centre Director, TIFR Hyderabad)

S. Ramakrishnan (Director, TIFR Mumbai)

**09:45 - 11:50 AM**

**Session Chair: G. Rajalakshmi**

V. Chandrasekhar

Single-ion Magnets Containing Lanthanide and Transition Metal ions

**09:45 - 10:10 AM**

Vamsee Voora

A Density Functional Approximation for Anionic States

**10:10 - 10:35 AM**

Pabitra K. Nayak

Adduct-based p-doping of Organic Semiconductors

**10:35 - 11:00 AM**

Soumya Ghosh

Computational electrochemistry: Metal-water interface under constant applied bias

**11:00 - 11:25 AM**

Vivek Polshettiwar

Capturing CO<sub>2</sub> Before its Release

**11:25 - 11:50 AM**

**BREAK**

**01:00 - 03:00 PM**

Poster presentation sessions (in parallel)

P1 - P12

P13 - P24

**BREAK**

**03:30-05:35 PM**

**Session Chair: Manoj V. Naik**

Malay Patra

Necrosis inducing hetero-bimetallic Pt(II)-Fe(II) derivatives overcome apoptosis resistance in cancer cells

**03:30 - 03:55 PM**

Arati Ramesh

Catch me if you can: A PHANTOM sensor to detect SARS-CoV-2

**03:55 - 04:20 PM**

Kalyaneswar Mandal

Blocking RBC invasion by malaria parasites using D-protein

**04:20 - 04:45 PM**

Pushpita Ghosh

Collective motions and emergent nonuniform spatiotemporal dynamics in active systems

**04:45 - 05:10 PM**

Ankona Datta

Designer Peptide-Based Sensors for Molecular Detection and Tracking

**05:10 - 05:35 PM**

**04 March 2021, Thursday**

**09:00-11:05 AM**

**Session Chair: Mamata V. Joshi**

Shruti Viswanath <b>09:00 - 09:25 AM</b>	Integrative structure of desmosomal plaques
Sri Rama Koti Ainavarapu <b>09:25 - 09:50 AM</b>	Azurin: Reconstruction, Structure and Dynamics
Jagannath Mondal <b>09:50 - 10:15 AM</b>	Molecular View of Biomimetic peptide in Action with Membrane
Shyamalava Mazumdar <b>10:15 - 10:40 AM</b>	Towards the Design of Hybrid Bio-catalysts by Engineering of Metalloproteins
Anand Vaidya <b>10:40 - 11:05 AM</b>	RNA stabilization by poly(A) tail triple helix and novel RNA-RNA interactions

**BREAK**

**11:30 - 01:00 PM**

Poster presentation sessions (in parallel)

P25 - P33 | P34 - P42

**BREAK**

**02:00-04:00 PM**

**ChemQuiz**

**Session In charge: Anand Vaidya**

**BREAK**

**04:30-07:00 PM**

**Looking back at Sanjay Wategaonkar's illustrious career in chemical sciences research**

**Session Chair: Shyamalava Mazumdar**

Pranav Shirhatti <b>04:30 - 04:55 PM</b>	Developing tools for studying quantum state resolved reaction dynamics
G. Naresh Patwari <b>04:55 - 05:20 PM</b>	Outer Valence Intermolecular Coulombic Decay
M. Krishnamurthy <b>05:20 - 05:45 PM</b>	Big issues with small clusters
<b>05:45 - 07:00 PM</b>	Felicitations of Sanjay Wategaonkar

**05 March 2021, Friday**
**09:00-11:05 AM**
**Session Chair: Deepa S.**

Sudipta Maiti <b>09:00 - 09:25 AM</b>	Probing toxic protein oligomers: From test tubes to patient-derived neurons
Shachi Gosavi <b>09:25 - 09:50 AM</b>	Understanding the folding of proteins which switch conformations.
Kanchan Garai <b>09:50 - 10:15 AM</b>	ATP independent inhibition of amyloid aggregation by Hsp70
Vinothkumar Kutti Ragunath <b>10:15 - 10:40 AM</b>	CryoEM structures of Dimethylformamidase
Kaustubh R. Mote <b>10:40 - 11:05 AM</b>	Studying dynamics using NMR at fast MAS frequencies

**BREAK**
**11:30 - 01:00 PM**

Poster presentation sessions (in parallel)

P43 - P50

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P51 - P58

**BREAK**
**02:00-03:00 PM**
**ChemFun Talk – 1 : Chemistry of Footwear / ChemFun Talk – 2 : The Art of Chemistry**
**Session Chair: Soumya Ghosh**
**BREAK**
**03:30-06:00 PM**
**Session Chair: D. Krishnarao**

Sanjay Wategaonkar <b>03:30 - 03:55 PM</b>	C-H---S Interaction Exhibits all the Characteristics of Conventional Hydrogen Bonds
Jyotishman Dasgupta <b>03:55 - 04:20 PM</b>	Probing Polarons in Conjugated Polymers using Broadband Femtosecond Absorption and Vibrational Spectroscopy
Deepa Khushalani <b>04:20 - 04:45 PM</b>	Simultaneous Water Splitting and CO <sub>2</sub> conversion in One Electrochemical Reaction
T. N. Narayanan <b>04:45 - 05:10 PM</b>	Role of Electrode-Electrolyte Interface Engineering in Electrodeics
Ravindra Venkatramani <b>05:10 - 05:35 PM</b>	Molecular Breadboard Circuits: Challenges and Prospects
Anukul Jana <b>05:35 - 06:00 PM</b>	Low-Valent Low-Coordinate Main-Group Compounds as Emerging New Class of Synthons
<b>06:00 - 06:15 PM</b>	<b>Concluding Remarks:</b>
Session In charge:	Smarajit Karmakar (Coordinator – Academics, TIFR Hyderabad)
Pramodh Vallurupalli	Surajit Sengupta (Dean, TIFR Hyderabad)
	Kalobaran Maiti (Dean – NSF, TIFR Mumbai)
	V. Chandrasekhar (Centre Director, TIFR Hyderabad)