<table>
<thead>
<tr>
<th>Time duration</th>
<th>Day 1: Thursday, February 22nd, 2018</th>
</tr>
</thead>
<tbody>
<tr>
<td>13:30-15:20</td>
<td><strong>Lunch</strong></td>
</tr>
<tr>
<td>15:25-15:30</td>
<td>Welcome by Prof Satrajit Adhikari, Head of the Department. of Physical Chemistry, IACS</td>
</tr>
<tr>
<td>15:30-15:45</td>
<td>Address by Prof. Debasish Mukherjee Indian Association for the Cultivation of Science, Kolkata</td>
</tr>
<tr>
<td><strong>15:45-17:15</strong></td>
<td>Technical Session I: Chair: Prof. S. P. Bhattacharyya (IACS)</td>
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<tr>
<td>15:45-16:20</td>
<td>Perspective talk by Prof. Santanu Bhattacharya Director, Indian Association for the Cultivation of Science</td>
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<tr>
<td>16:20-16:55</td>
<td>Perspective talk by Prof. Sourav Pal Director, Indian Institute of Science Education and Research Kolkata</td>
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<tr>
<td>16:55-17:15</td>
<td>Prof. Sotir Chervenkov (Max Planck Institute of Quantum Optics, Munich, Germany) Slowing down of molecules</td>
</tr>
<tr>
<td><strong>17:15-18:00</strong></td>
<td><strong>Tea Break</strong></td>
</tr>
<tr>
<td><strong>18:00-19:30</strong></td>
<td>Technical Session II: Chair: Prof. Sanjib Ghosh (Adamas University, Kolkata)</td>
</tr>
<tr>
<td>18:00-18:20</td>
<td>Prof. Samir Pal (SNBNCBS) <em>The Key Spectroscopy for the Development of Indigenous Technology</em></td>
</tr>
<tr>
<td>18:20-19:00</td>
<td>Perspective talk by Prof. Siva Umapathy Indian Institute of Science, Bangalore <em>Ultrafast Raman spectroscopy: Applications to chemical dynamics</em></td>
</tr>
<tr>
<td><strong>19:00-</strong></td>
<td><strong>Dinner</strong></td>
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<tr>
<td>Time duration</td>
<td>Day 2: Friday, February 23rd, 2018</td>
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<tr>
<td>10:00-11:40</td>
<td>Technical Session III: Chair: Prof. Tapanendu Kundu (IIT Bombay)</td>
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<tr>
<td></td>
<td><strong>Speaker</strong></td>
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<tr>
<td>10:00-10:20</td>
<td>Chayan K. Nandi (IIT Mandi)</td>
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<tr>
<td>10:20-10:40</td>
<td>Prasun Mandal (IISER Kolkata)</td>
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<tr>
<td>10:40-11:00</td>
<td>Anindya Datta (IITB Mumbai)</td>
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<tr>
<td>11:25-11:40</td>
<td>Sayan Bagchi (NCL Pune)</td>
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<td>11:40-12:00</td>
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<tr>
<td>12:00-13:30</td>
<td>Technical Session IV: Chair: Dr. Ruchi Anand (IIT Bombay)</td>
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<tr>
<td>12:00-12:20</td>
<td>Dilip K. Maity (BARC, Mumbai)</td>
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<tr>
<td>12:20-12:40</td>
<td>Ashwani K. Tiwari (IISER Kolkata)</td>
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<tr>
<td>12:40-12:55</td>
<td>Sumana Dutta (IITG, Guwahati)</td>
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<tr>
<td>12:55-13:10</td>
<td>Viola C. Dmello (TIFR Mumbai)</td>
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<tr>
<td>13:10-13:30</td>
<td>Saurabh Nagpal (Agilent Technologies)</td>
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<td>13:30-15:00</td>
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<td>15:00-16:45</td>
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<td>Time</td>
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<tr>
<td>16:00-16:45</td>
<td><strong>Tea will be served</strong></td>
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<tr>
<td>17:00-18:50</td>
<td><strong>Technical Session VI:</strong> Chair: Prof. Kamal Bhattacharyya (University of Calcutta) and Prof. Sanjib Bagchi (Presidency University)**</td>
</tr>
<tr>
<td>17:00-17:30</td>
<td>Perspective talk by Prof. Deb Shankar Ray</td>
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<tr>
<td></td>
<td>Indian Association for the Cultivation of Science, Kolkata</td>
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<tr>
<td></td>
<td><em>Pattern formation in non-equilibrium systems</em></td>
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<tr>
<td>17:30-18:00</td>
<td>Perspective talk by Prof. Sudipta Maity</td>
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<tr>
<td></td>
<td>Tata Institute of Fundamental Research, Mumbai</td>
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<tr>
<td></td>
<td><em>Dynamics Guided Ligand Design for Disordered Proteins</em></td>
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<tr>
<td>18:00-18:25</td>
<td>Prof. G. Naresh Patwari (IIT B, Mumbai)</td>
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<tr>
<td></td>
<td><em>Do Supramolecular Synthons Defy Two Body Interactions?</em></td>
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<tr>
<td>18:25-18:40</td>
<td>Dr. K. R. Shamasundar (IISER Mohali)</td>
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<td></td>
<td><em>Diagonal Born-Oppenheimer Correction for Coupled-Cluster Wave-functions</em></td>
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<tr>
<td>18:40-</td>
<td><strong>Dinner</strong></td>
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**Day 3: Saturday, February 24th, 2018**

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
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<tbody>
<tr>
<td>10:00-11:45</td>
<td><strong>Technical Session VII: Chair: Prof. Puspendu K. Das (IISc. Bangalore)</strong></td>
</tr>
<tr>
<td>10:00-10:20</td>
<td>Dr. Pujarini Banerjee (IACS), summarizes scientific contribution of Prof. Sanjay Wategaonkar, TIFR, Mumbai</td>
</tr>
<tr>
<td><strong>Speaker</strong></td>
<td><strong>Title of the Talk</strong></td>
</tr>
<tr>
<td>10:20-10:45</td>
<td>Rajesh K.Vatsa (BARC, Mumbai)</td>
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<tr>
<td></td>
<td><em>Gigawatt Pulse Driven Coulomb Explosion in van der Waals Clusters</em></td>
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<tr>
<td>10:45-11:10</td>
<td>B. Rajakumar (IIT M)</td>
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<tr>
<td></td>
<td><em>Gas Phase Kinetics and Spectroscopy Relevant to Atmospheric and Combustion Processes</em></td>
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<tr>
<td>11:10-11:30</td>
<td>Aloke Das (IISER Pune)</td>
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<td></td>
<td><em>Gas phase IR spectroscopic signature for C=O...C=O n→π</em> interactions in the building block of collagen*</td>
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<tr>
<td>11:30-11:45</td>
<td>Arijit Das (IISc Bangalore)</td>
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<td></td>
<td><em>Rotational Spectra of H2S Dimer: Observation of K_a=1 Lines</em></td>
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<tr>
<td>Time</td>
<td>Session Title</td>
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<td>11:35-12:00</td>
<td><strong>Tea Break</strong></td>
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<tr>
<td>12:00-13:25</td>
<td><strong>Technical Session VIII</strong>; Chair: Prof. Rajat Chaudhuri (IIAP, Bangalore)</td>
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<td>12:55-13:00</td>
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<tr>
<td>13:15-15:00</td>
<td><strong>Lunch</strong></td>
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<tr>
<td>15:00-17:00</td>
<td><strong>Technical Session IX</strong>; Chair: Prof. Mintu Halder (IIT Kharagpur)</td>
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<tr>
<td>15:00-15:20</td>
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<td>15:35-15:50</td>
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<td>16:05-16:20</td>
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<td>16:20-16:35</td>
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<tr>
<td>16:35-17:00</td>
<td><strong>Tea break</strong></td>
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<tr>
<td>Time</td>
<td>Session Title</td>
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<tr>
<td>17:00-19:00</td>
<td>Technical Session X: Prof. Nitin Chattopadhyay (JU) and Prof. Nikhil Gucchait (CU)</td>
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<td>17:00-17:30</td>
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<td>17:30-17:50</td>
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<td>18:45-19:00</td>
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<tr>
<td>19:10-</td>
<td><strong>Dinner</strong></td>
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**Day 4: Sunday, February 25th, 2018**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Title</th>
<th>Speaker</th>
<th>Title of talk</th>
</tr>
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<tbody>
<tr>
<td>10:00-11:30</td>
<td>Technical Session XI: Chair: Dr. Arindam Chowdhury (IIT Bombay)</td>
<td>Pradipta Purkayastha (IISER Kolkata)</td>
<td>Small Molecule Interactions with Lipid Vesicles: FLIM and FCS Outcomes</td>
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<tr>
<td>10:00-10:15</td>
<td></td>
<td>Debarati Ray (CU, Kolkata)</td>
<td>Lactim-Lactam Tautomerism on Gold Nanosurface</td>
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<tr>
<td>10:15-10:30</td>
<td></td>
<td>Saptarsi Mondal (IACS)</td>
<td>Role of Dispersive Fluorous Interaction in the Photophysics And Solvation Dynamics of the Perfluoro Group Containing Molecules</td>
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<tr>
<td>Time</td>
<td>Presenter/Institution</td>
<td>Topic</td>
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<tr>
<td>10:45-11:00</td>
<td>Ishita Das (IITKGP)</td>
<td>pH dependent interaction of norfloxacin housed in lysozyme: The protein modulates the prototropic equilibrium of the drug to host the preferred ionized state</td>
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<tr>
<td>11:00-11:15</td>
<td>Avijit Shee (Univ. of Michigan)</td>
<td>GW method using the Cholesky decomposition technique with applications to QM/QM embedding approaches</td>
<td></td>
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<tr>
<td>11:15-11:30</td>
<td>Srijee Talukder (IACS Kolkata)</td>
<td>Getting selective bond dissociation in triatomic molecules by optimally designed polychromatic pulse: A stochastic optimization based study</td>
<td></td>
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<tr>
<td>11:30-12:00</td>
<td></td>
<td>Tea Break</td>
<td></td>
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<tr>
<td>12:00-13:00</td>
<td><strong>Technical Session XII:</strong> Chair: Prof. Debasis Mukhopadhyay (CU)</td>
<td></td>
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<tr>
<td>12:00-12:15</td>
<td>Bidhan C. Bag (Visva Bharati)</td>
<td>Bounds of the entropy production of the irreversible thermodynamics and its relation with the non-equilibrium temperature</td>
<td></td>
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<tr>
<td>12:15-12:30</td>
<td>Biplab Sarkar (NEHU)</td>
<td>Hydrogen bonding interactions in gas phase 3-halo catechol and 2-hydroxy thiophenol with a water molecule</td>
<td></td>
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<tr>
<td>12:30-12:45</td>
<td>Pulak K. Ghosh (Presidency Univ.)</td>
<td>Transport properties of artificial micro-swimmers in periodic structures</td>
<td></td>
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<tr>
<td>12:45-13:00</td>
<td>Anirban Karmakar (SNBNCBS, Kolkata)</td>
<td>Molecular Conductance through pyridine system</td>
<td></td>
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<tr>
<td>13:00-13:15</td>
<td>Pujarini Banerjee (IACS Kolkata)</td>
<td>Matrix isolation IR spectroscopy of strong (O-H···O) and weakly bound (O-H···π) binary H-bonded complexes: Origin of donor νO-H shift</td>
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<tr>
<td>13:15-14:30</td>
<td></td>
<td>Lunch</td>
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<tr>
<td>14:30-15:50</td>
<td><strong>Technical Session XIII:</strong> Chair: Prof. Debashis Mukherjee (IACS)</td>
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<tr>
<td>14:30-14:50</td>
<td>Bimalendu Deb (IACS Kolkata)</td>
<td>Ion-atom Cold Collisions and Photoassociations</td>
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<tr>
<td>15:10-15:30</td>
<td>Ayan Datta (IACS Kolkata)</td>
<td>Singlet Fission in Organic Molecular Crystals-Molecular Pathways</td>
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<tr>
<td>Time</td>
<td>Speaker</td>
<td>Title</td>
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<tr>
<td>15:30-15:50</td>
<td>Debashree Ghosh (IACS Kolkata)</td>
<td>Photo-processes in biological systems – Need for hybrid QM/MM with polarization</td>
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<tr>
<td>15:50-16:15</td>
<td></td>
<td><strong>Tea Break</strong></td>
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<tr>
<td>16:15-17:35</td>
<td><strong>Technical Session XIV:</strong> Prof. Pinaki Chaudhury (CU) and Prof. Gautam Gangopadhyay (SNBNCBS)</td>
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<tr>
<td>16:15-16:35</td>
<td>Ravindra Pandey (IACS Kolkata)</td>
<td>In Situ Probing of Charge Transfer States at Buried Organic Interfaces with Even-Order Spectroscopy</td>
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<tr>
<td>16:35-16:55</td>
<td>Bidisa Das (IACS Kolkata)</td>
<td>Theoretical Study of Small Iron-oxyhydroxide Clusters and Formation of Ferrihydrite</td>
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<tr>
<td>16:55-17:15</td>
<td>Avishek Das (IACS Kolkata)</td>
<td>Multiscale simulation of conformational dynamics of an ATP-driven calcium transporting membrane protein</td>
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<tr>
<td>17:15-17:35</td>
<td>Biman Jana (IACS Kolkata)</td>
<td>Decoding the Unusual Structure of an antifreeze protein: Implications from Low Temperature Hydrophobicity</td>
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