

**Schedule of the Workshop**  
**“Multiscale Modeling and Simulation”**  
**2<sup>nd</sup> April to 6<sup>th</sup> April 2018**

<b>2<sup>nd</sup> April Monday</b>	<b>3<sup>rd</sup> April Tuesday</b>	<b>4<sup>th</sup> April Wednesday</b>	<b>5<sup>th</sup> April Thursday</b>	<b>6<sup>th</sup> April Friday</b>
9.00 to 10:00 Registraton and Breakfast	9.00 to 9:45 Breakfast	9.00 to 9:45- Breakfast	9.00 to 9:45 Breakfast	8.30 to 9:00- Breakfast
10.00 to 11.30 <b>Inauguration</b> and Talk: Theoretical and Computational Chemistry: A Brief Historical Perspective- <b>Prof. Sridhar Gadre, SPPU, Pune</b>	9.45 to 11.15 Talk: Molecular Dynamics Simulation and Its Appl. <b>Ahmed Sayeed, SPPU, Pune</b>	9.45 to 11.15 Talk: Hartree-Fock theory <b>Prof. Sridhar Gadre SPPU, Pune</b>	9.45 to 11.15 Talk on Density Functional Theory Dr. Kavita Joshi, NCL	9.00 to 10.30 Density Functional Theory Dr. Kavita Joshi, NCL
11.30 to 11.45 Tea	11.15 to 11.30 - Tea	11.15 to 11.30 - Tea	11.15 to 11.30- Tea	10.30 to 10.45- Tea
11.45 to 13.00 Talk: Complexity in Modeling and Simulation: Two case studies (Micro-fluidic devices and Electrophoretic deposition process) <b>Dr. Sukratu Barve SPPU, Pune</b>	11.30 to 13.00 Talk: Molecular Dynamics Simulation and Its Appl. <b>Dr. Ahmed Sayeed, SPPU, Pune</b>	11.30 to 13.00 Talk: Treating Large molecules by ab initio methods: an art of the possible <b>Prof. Sridhar Gadre SPPU, Pune</b>	11.30 to 13.00 Talk on Density Functional Theory Dr. Kavita Joshi, NCL	10.45 to 12.15 Density Functional Theory Dr. Kavita Joshi, NCL
13.00 to 14.00 Lunch	13.00 to 14.00 Lunch	13.00 to 14.00 Lunch	13.00 to 14.00 Lunch	12.15 to 13.00 Lunch
14:00 to 15:30 Talk: Reducing Complexity: Example of Application of M&S Principles (Tank Weapons Systems) <b>Dr. Sukratu Barve SPPU, Pune</b>	14:00 to 15:30 Lab: Molecular Dynamics Simulation and Its Appl. <b>Dr. Ahmed Sayeed, SPPU, Pune</b>	14:00 to 15:30 Lab Session by <b>Mr. Subodh Khire SPPU, Pune</b>	14:00 to 15:30 Density Functional Theory Lab Session by Dr. Kavita Joshi, NCL	13:00 to 15:30 Density Functional Theory Lab Session by Dr. Kavita Joshi, NCL
15:30 to 15:45 Tea	15:30 to 15:45 Tea	15:30 to 15:45 Tea	15:30 to 15:45 Tea	15:30 to 15:45 Tea
15:45 to 17:15 Talk: Theory of Devices- A Framework for Handshaking Down from Macro Scales <b>Dr. Sukratu Barve SPPU, Pune</b>	15:45 to 17:15 Lab: Molecular Dynamics Simulation and Its Appl. <b>Dr. Ahmed Sayeed, SPPU, Pune</b>	15:45 to 17:15 Lab Session by <b>Mr. Subodh Khire SPPU, Pune</b>	15:45 to 17:15 Density Functional Theory Lab Session by Dr. Kavita Joshi, NCL	15.30 to 5.30 Valedictory Function

