

Scientific Program Schedule

The 7th International Conference on Molecular Simulation (ICMS 2026)

4-8 October 2026 | J. N. Tata Auditorium, Indian Institute of Science, Bengaluru

- **Talk durations:** Plenary 40 min; **Keynote 30 min; Invited 20 min; Contributed 15 min**
- **Number of Talks:** 6 Plenary; **22 Keynote; 79 Invited; 60 Contributed**
- **Parallel themes:**
 - Biological Systems and Medicine (6 sessions)
 - Catalysis and Surface Science (3 sessions)
 - Computational Material Sciences (3 sessions)
 - Machine Learning and AI, and Molecular Modeling (6 sessions)
 - Theory and Methodology (3 sessions)
 - Polymers and Soft Matter (4 sessions)
 - Energy (1 session)
 - Materials and Biological Systems (1 session).

Sunday, 4 October 2026

Time	J. N. Tata Auditorium
16:00-19:00	REGISTRATION AND KIT DISTRIBUTION
17:00-19:00	WELCOME RECEPTION

Monday, 5 October 2026

Time	Main Auditorium	Hall A	Hall B	Hall C
08:00-09:00	REGISTRATION			
09:00-09:30	INAUGURATION / WELCOME ADDRESS – Main Auditorium			
09:30-10:10	PLENARY LECTURE I – Main Auditorium J. Ilja. Siepmann, University of Minnesota, Minneapolis, USA (Chair: Ganapathy Ayappa)			
10:10-10:30	Tea break			
10:30-12:30	Parallel Session I Biological Systems and Medicine Chair: Nobuyuki Matubayasi Keynote Talk: Florence Tama Invited Talk: Jun Soo Kim Invited Talk: Ricky Nellas Contributed Talk: Arvinpreet Kaur Contributed Talk: Stefan Hervø-Hansen Contributed Talk: Sudipto Muhuri	Parallel Session I Computational Material Sciences Chair: Jayant K Singh Keynote Talk: Shiang-Tai Lin Invited Talk: Bong June Sung Invited Talk: Priya Johari Contributed Talk: Unity Ekugbe Oluwaiye Contributed Talk: Sahane Nisha Contributed Talk: Chaitanya Jitendra Shah	Parallel Session I ML/AI and Molecular Modeling Chair: Balasubramanian Sundaram Keynote Talk: Jhih-Wei Chu Invited Talk: Kaito Takahashi Invited Talk: Anirban Mondal Contributed Talk: Sridip Parui Contributed Talk: Karan Deep Sharma	Parallel Session I Catalysis and Surface Science Chair: Lisa Roy Keynote Talk: Hyungjun Kim Invited Talk: Ateeque Malani Invited Talk: Anil Boda Contributed Talk: Minh M. Kim Contributed Talk: Naiwrit Karmodak Contributed Talk: Jaewoo Jeong
12:30-14:00	LUNCH			
14:00-14:40	PLENARY LECTURE II – Main Auditorium Amalendu Chandra, Indian Institute of Technology Kanpur, India (Chair: Hyungjun Kim)			
14:40-15:00	TEA BREAK			
15:00-17:00	Parallel Session II Biological Systems and Medicine Chair: Manoj Varma Keynote Talk: Garima Jindal Invited Talk: Yuan-Chung Invited Talk: Sudip Das Invited Talk: Abhishek Sirohiwal Contributed Talk: Aditya Kumar Contributed Talk: Sangeetha Balasubramanian	Parallel Session II Theory and Methodology Chair: Amalendu Chandra Keynote Talk: Nisanth N Nair Invited Talk: Shinji Saito Invited Talk: Phani Motamarri Invited Talk: Susmita Roy Contributed Talk: Ryoma Sasaki Contributed Talk: Praveen Kumar Bommineni	Parallel Session II Polymers and Soft Matter Chair: Neelanjana Sengupta Keynote Talk: Nobuyuki Matubayasi Invited Talk: Takahiro Murashima Invited Talk: Debayan Chakraborty Invited Talk: BL Bhargava Contributed Talk: Takahiro Koishi Contributed Talk: Shubham Kumar	Parallel Session II Energy Chair: Hemant Kumar Invited Talk: Abhishek Aggarwal Invited Talk: Lukman Hakim Invited Talk: Yoshitaka Tateyama Invited Talk: Arun Venkatnathan Contributed Talk: Dhileep Nagi Reddy Thummuru Contributed Talk: Srikanth Divi
17:00-19:00	POSTER SESSION I + High Tea			

Tuesday, 6 October 2026

Time	Main Auditorium	Hall A	Hall B	Hall C
09:30-10:10	PLENARY LECTURE III – Main Auditorium Sang Soo Han, KIST, South Korea (Chair: Prabal Maiti)			
10:10-10:30	TEA BREAK			
10:30-12:30	Parallel Session III Biological Systems and Medicine Chair: Anand Srivastava Keynote Talk: Durba Sengupta Invited Talk: Min-Yeh Tsai Invited Talk: Ai Niitsu Contributed Talk: Aswin Vinod M Contributed Talk: Rajalakshmi Chockalingam Contributed Talk: Debabrata Pramanik	Parallel Session III Computational Material Sciences Chair: Subir Das Keynote Talk: Ananya Debnath Invited Talk: Vladimir Stegailov Contributed Talk: Swagata Pahari Contributed Talk: Sachin Aditya Ramesh Contributed Talk: Meena Devi J Contributed Talk: Binu Varghese	Parallel Session III ML/AI and Molecular Modeling Chair: Jagannath Mondal Keynote Talk: Jer-Lai Kuo Invited Talk: Jack Evans Invited Talk: Kartik Sau Invited Talk: Musharaf Ali Sheikh Contributed Talk: Jihoo Kim Contributed Talk: Swathi Srinivasan	Parallel Session III Theory and Methodology Chair: Florence Tama Keynote Talk: Alan Mark Invited Talk: Tod Pascal Invited Talk: Shinichi Miura Invited Talk: Sudeep Punnathanam Contributed Talk: Suvadip Das Contributed Talk: Manas Sharma
12:30-14:00	Lunch			
14:00-14:40	PLENARY LECTURE IV – Main Auditorium Yuji Sugita, RIKEN, Japan (Chair: Ananth Govind Rajan)			
14:40-15:00	TEA BREAK			
15:00-17:00	Parallel Session IV Biological Systems and Medicine Chair: R. Venkatramani Keynote Talk: Ganapathy Ayappa Invited Talk: Toshifumi Mori Invited Talk: Padmesh Anjukandi Invited Talk: Arnab Mukherjee Contributed Talk: Milan Kumar Hazra Contributed Talk: Sanjoy Paul	Parallel Session IV ML/AI and Molecular Modeling Chair: Jer-Lai Kuo Keynote Talk: Yousung Jung Invited Talk: Sungwoo Kang Invited Talk: Balasubramanian Sundaram Invited Talk: Dibyajyoti Ghosh Contributed Talk: Dr. Ravi Kumar Reddy Addula	Parallel Session IV Polymers and Soft Matter Chair: Bong June Sung Keynote Talk: Takeshi Kawasaki Invited Talk: Prateek Jha Invited Talk: YongJoo Kim Invited Talk: Yves Lansac Invited Talk: Kazushi Fujimoto	Parallel Session IV Catalysis and Surface Science Chair: Swapan Pati Invited Talk: Tej Choksi Invited Talk: Nitish Govindarajan Invited Talk: Akira Nakayama Contributed Talk: Debdeep Bhandary Contributed Talk: Aravindhan Ramachandran
17:00-19:00	POSTER SESSION II + High Tea (18:00-18:45: International Advisory Committee Meeting)			
19:00-21:30	CONFERENCE BANQUET			

Wednesday, 7 October 2026

Time	Main Auditorium	Hall A	Hall B	Hall C
09:30-10:10	PLENARY LECTURE V – Main Auditorium Satyavani Vemparala, The Institute of Mathematical Sciences, Chennai, India (Chair: Durba Sengupta)			
10:10-10:30	TEA BREAK			
10:30-12:30	Parallel Session V Biological Systems and Medicine Chair: Arnab Mukherjee Keynote Talk: Wataru Shinoda Invited Talk: Shachi Gosavi Invited Talk: Srabani Taraphder Invited Talk: Himanshu Joshi Contributed Talk: Subbarao Kanchi Contributed Talk: Abhinava Chatterjee	Parallel Session V ML/AI and Molecular Modeling Chair: Musharaf Ali Sheikh Keynote Talk: Guan Hua Chen Invited Talk: Jagannath Mondal Invited Talk: Shelaka Gupta Invited Talk: Biman Jana Contributed Talk: Kumari Soniya Contributed Talk: Yogendra Kumar	Parallel Session V Polymers and Soft Matter Chair: Prasenjit Sen Keynote Talk: Yun Hee Jang Invited Talk: Neelanjana Sengupta Invited Talk: Kun-Han Lin Invited Talk: Shibananda Das Contributed Talk: Prateek Chowdhury Contributed Talk: Vrinda Garg	Parallel Session V Catalysis and Surface Science Chair: Padma Kumar Padmanabhan Keynote Talk: Nikos Doltsinis Invited Talk: Ananth Govind Rajan Invited Talk: Lisa Roy Contributed Talk: Dr. Aritri Biswas Contributed Talk: Jijo Johnson
12:30-14:00	LUNCH			
14:00-14:40	PLENARY LECTURE VI – Main Auditorium Roland Netz, FU Berlin, Germany (Chair: Sudeep Punathanam)			
14:40-15:00	TEA BREAK			
15:00-17:00	Parallel Session VI Polymers and Soft Matter Chair: Prateek Jha Invited Talk: Sutapa Roy Invited Talk: Sanjay Kumar Invited Talk: Jure Dobnikar Invited Talk: Nirmalya Bachhar Invited Talk: Kang Kim Contributed Talk: Jayeeta Chattopadhyay	Parallel Session VI ML/AI and Molecular Modeling Chair: Ananya Debnath Keynote Talk: Supawadee Namuangruk Invited Talk: Hemant Kumar Invited Talk: Prasenjit Sen Invited Talk: Sai Gautam Invited Talk: Gopalakrishnan Contributed Talk: Mithun Biswas Contributed Talk: Varad Daoo	Parallel Session VI Theory and Methodology Chair: Ateeque Malani Invited Talk: Debashree Chakraborty Invited Talk: Susumu Okazaki Invited Talk: Santosh Mogurampelly Invited Talk: Kento Kasahara Invited Talk: Ravindra Venkatramani Contributed Talk: Anil Kumar Sahoo	Parallel Session VI Industry / Special Session Chair: Ananth Govind Rajan Invited Talk: Somananda Sanyal, Wiley Invited Talk: Ritwik Kavathekar, Biovia, Dassault Systemes Invited Talk: Ashutosh, Micropoint Computers Pvt. Ltd. Invited Talk: National Program on Technology Enhanced Learning (NPTEL)
17:00-19:00	POSTER SESSION III + High Tea			

Thursday, 8 October 2026

Time	Main Auditorium	Hall A	Hall B	Hall C
09:30-11:30	Parallel Session VII Biological Systems and Medicine Chair: Shinji Saito Keynote Talk: Anand Srivastava Invited Talk: Ramasubbu Sankararamakrishnan Invited Talk: Aditya Padhi Invited Talk: Prapasiri Pongprayoon Contributed Talk: Raj Kumar Sadhu Contributed Talk: Amar Krishna Gopinath	Parallel Session VII Computational Material Sciences Chair: Sai Gautam Gopalakrishnan Keynote Talk: Jayant K Singh Invited Talk: Sairam Mallajosyula Invited Talk: Krishan Kanhaiya Contributed Talk: Ravi C. Dutta Contributed Talk: Diksha Kadre Contributed Talk: Prashil Badwaik	Parallel Session VII ML/AI and Molecular Modeling Chair: Yun Hee Jang Keynote Talk: Sanjib Senapati Invited Talk: Saientan Bag Invited Talk: Tarak Patra Invited Talk: RS Swathi Contributed Talk: Maida Engels SE Contributed Talk: Arya Das	Parallel Session VII Materials and Biological Systems Chair: Supawadee Namuangruk Contributed Talk: Sayari Bhattacharya Contributed Talk: Rakesh K Vaiwala Contributed Talk: Pooja Sahu Contributed Talk: V N Ravi Kishore Vutukuri Contributed Talk: Pujarini Mahapatra Contributed Talk: Sayantan Maity
11:30-12:30	CONCLUSION SESSION – MAIN AUDITORIUM			
12:30-14:00	LUNCH/DEPARTURE			