CM4 2026

International Conference on Computational and Machine Learning Modelling of Molecules and Materials

Club Mahindra Poovar, Thiruvananthapuram, Kerala, India
3–6 December 2026 · https://www.cm4-2026.org · All times IST

Thursday, 3 December 2026 | 3–6 DECEMBER 2026

TIME	SESSION / SPEAKER DETAILS
13:00–14:00	**Registration**
14:15–14:45	**Inaugural Session**
14:45–16:15	**Opening lectures** | SESSION CHAIR | **Prof. Bharatam V. Prasad, NIPER Mohali**
14:45–15:30	**Sason Shaik**, Hebrew University of Jerusalem *Oriented Electric Fields - Universal Catalysts (online)*
15:30–16:15	**Henry F. Schaefer III**, University of Georgia *Professor E. D. Jemmis: A Career of Great Scientific Distinction*
16:15–16:45	TEA
16:45–17:50	SESSION CHAIR | **Soujanya Yarasi, CSIR-IICT**
16:45–17:10	**N. Arul Murugan**, IIIT Delhi *Physics-Based and Data-Driven Approaches for Drug-like Property Prediction*
17:10–17:35	**Arjun Ray**, IIIT Delhi *Cross-family prediction of receptor agonism and antagonism with PAIR*
17:35–17:50	**Anjalin Joy**, IIT Palakkad *Flavin-Mediated Oxidation of Cholesterol and its Subsequent Isomerization: Insights from Cholesterol Oxidase Inspired Models*
17:50–18:50	**Poster Session I** SESSION CHAIR | **Sherin D. R., Digital University Kerala** Posters P01–P09: see poster list
19:00–21:00	DINNER

Friday, 4 December 2026 | 3–6 DECEMBER 2026

TIME	SESSION / SPEAKER DETAILS
09:00–10:30	SESSION CHAIR | **Priyakumari C. P., IISER Mohali**
09:00–09:45	**V. Subramanian**, SRM Institute of Science and Technology *Design and Development of Carbon based Two-Dimensional Materials and their Applications*
09:45–10:10	**Ashim Nandi**, IIT Goa *From Chemical Reactivity to Drug Design: Mechanistic Insights into Covalent Inhibition*
10:10–10:25	**Saikat Roy**, University of Warsaw *Autoionizing Rydberg states in atoms and molecules as a stringent test of quantum-chemical theory*
10:25–10:30	DISCUSSION
10:30–11:00	TEA
11:00-12:50	SESSION CHAIR | **Biswarup Pathak, IIT Indore**
11:00–11:45	**Satoshi Maeda**, WPI-ICReDD, Hokkaido University *Ab Initio Chemical Reaction Discovery via a Force-Based Algorithm*
11:45–12:10	**Akhil S. Nair**, CSIR–Indian Institute of Chemical Technology, Hyderabad *Towards High-Fidelity General-Purpose Machine-Learning Force Fields for Materials*
12:10–12:35	**Étienne Derat**, Sorbonne Université / CNRS *Understanding selectivities in radical reaction: the case of Truce–Smiles rearrangement*
12:35–12:50	**Sandeep Kumar**, Applied Materials India, Bengaluru *Surface Engineering for Atomic Layer Deposition*
12:50–13:05	BREAK BEFORE LUNCH
13:05–14:00	LUNCH
14:00–15:50	SESSION CHAIR | **P. Parameswaran, NIT Calicut**
14:00–14:45	**Odile Eisenstein**, ICGM, Université de Montpellier / CNRS / ENSCM; University of Oslo *Bridging Computation and Experiment for organomagnesium and organolithium complexes (online)*
14:45–15:10	**Amitabha Das**, NIT Mizoram *Single Atom Doped Interface Catalyst for the Selective CO_2 Conversion to C_2 Products*

TIME	SESSION / SPEAKER DETAILS
15:10–15:35	**R. S. Swathi**, IISER Thiruvananthapuram *Swarm Intelligence Guided Global Minima Search on Complex Potential Energy Surfaces*
15:35–15:50	**Sagar Ghorai**, ICReDD, Hokkaido University *Toward Reaction Vessel Mimicry: Machine Learning Assisted Automated Exploration of Alkene Polymerization and CO Coupling Reactions*
15:50–16:15	TEA
16:15–18:45	**Poovar Backwaters and Estuary Excursion**
19:15–21:00	DINNER

Saturday, 5 December 2026 | 3–6 DECEMBER 2026

TIME	SESSION / SPEAKER DETAILS
09:00–11:00	SESSION CHAIR | **E. G. Jayasree, CUSAT, Kochi**
09:00–09:45	**Krishnan Raghavachari**, Indiana University Bloomington *Approaching Coupled Cluster Accuracy at Density Functional Theory Cost Using Connectivity-Based Hierarchy and Machine Learning*
09:45–10:10	**Arup Mahata**, IIT Hyderabad *TBA*
10:10–10:35	**Subhendu Roy**, Saha Institute of Nuclear Physics, Kolkata *TBA*
10:35–10:50	**Dr. Surya K.**, IIT Palakkad *Catalyst–Substrate–Lewis Acid Templates Govern Regioselective Alkenylation and Alkylation of Pyridines*
11:00–11:30	TEA BREAK
11:30–13:30	SESSION CHAIR | **Dr. Madhavi Sastry, Schrödinger, India**
11:30–12:15	**Martin Zacharias**, Technical University of Munich *Biomolecular interaction modulation studied by ligand design and molecular simulations*
12:15–12:40	**Abhishek Sirohiwal**, Indian Institute of Science, Bengaluru *TBA*
12:40–13:05	**Padmesh Anjukandi**, IIT Palakkad *Unfavorable Chemistry and Towards its Stabilization and Utility*
13:05–13:20	**Souvik Sinha**, Prescience Insilico *From Computational Tools to Agentic AI: A Co-Scientist for Every Scientist*
13:20–13:30	DISCUSSION
13:30–14:00	LUNCH
14:00–15:30	SESSION CHAIR | **P. D. Pancharatna, Amrita Vishwa Vidyapeetham**
14:00–14:45	**Peter Comba**, Heidelberg University *Modeling Spin for Applications of Metal Complexes*

TIME	SESSION / SPEAKER DETAILS
14:45–15:10	**Upakarasamy Lourderaj**, NISER Bhubaneswar *Mechanisms and Dynamics of Bimolecular Nucleophilic Substitution Reactions at Nitrogen Centers*
15:10–15:25	**Pritam Chakraborty**, IIT Palakkad *Rational Design of an Anti-aromatic COFs Towards the Efficient Sequestration of Environmental and Biological Harmful Oxocarbons – A Comprehensive Theoretical Study*
15:25–15:30	DISCUSSION
15:30–17:00	**Poster Session II** SESSION CHAIR | **Susmita De, University of Calicut** Posters P10–P19: see poster list
17:00–17:45	**Special Scientific Lecture — E. D. Jemmis, Indian Institute of Science, Bengaluru** | Chair: U. Deva Priyakumar, IIIT Hyderabad *Recent Developments in three membered rings*
17:45–18:30	TEA BREAK AND PREPARATION FOR FELICITATION
18:30–20:00	**Felicitation Session | Chair: Prof. G. N. Sastry (IIT Hyderabad) & Dr. Dandamudi Usharani (CSIR-CFTRI)**
20:00–20:20	BREAK BEFORE GALA DINNER
20:20–22:00	GALA DINNER

Sunday, 6 December 2026 | 3–6 DECEMBER 2026

TIME	SESSION / SPEAKER DETAILS
09:00–10:35	SESSION CHAIR | **Prof. C. V. Sastri**
09:00–09:45	**T. P. Radhakrishnan**, University of Hyderabad *Heuristic Models for the Environment Sensitive Fluorescence Enhancement and Tuning in DADQ Molecules/Materials*
09:45–10:10	**Rositha Kuniyil**, IIT Palakkad *On the Role of Microenvironmental Effects in Catalytic Mechanisms*
10:10–10:35	**Subhas Ghosal**, NIT Durgapur *From Electronic Structure to Surface Protection: ML Modelling of Benzothiazole Corrosion Inhibitors*
10:35–11:00	TEA
11:00–11:50	SESSION CHAIR | **Prof. C. V. Sastri**
11:00–11:25	**Deb Ranjan Banerjee**, NIT Durgapur *3D-QSAR and Pharmacophore mapping: Two ML extensions to Anti-Alzheimer's Lead Discovery*
11:25–11:50	**Parthasarathi Ramakrishnan**, CSIR-HRDG, New Delhi *TBA*
11:50–11:55	**Poster Awards | Susmita De and Sherin D. R.**
11:55–12:10	**Valedictory and closing remarks**
12:15 onwards	DEPARTURE

Poster Session I

Thursday, 3 December 2026 | 17:50–18:50 IST

SESSION CHAIR | **Sherin D. R., Digital University Kerala**

P01 Navigating the Gold–Thiolate Energy Landscape with Chemically Informed Metal–Ligand Pair Growth
Sayan Paul — IIT Kharagpur

P02 Decoding Voltage in Organic Dual-Ion Batteries: A Combined DFT-Machine Learning Roadmap for Anode and Cathode Design
Poulami Paul — IIT Indore

P03 Stereoselective Identification of DNA Lesions: Quantum Transport Fingerprints Meet Machine Learning
Dipti Maurya — IIT Indore

P04 Transition state model for the Manganese Based chemical hydrogen battery
Krishnapriya A. U. — IIT Palakkad

P05 Amido N-Heterocyclic Carbenes: Electronic Properties and Synthesis
Govinddas M. Vaishnav — NIPER Mohali

P06 Nitreones: Theory, Synthesis and Drug Discovery
Sanjeev Ranjan — NIPER Mohali

P07 Adsorbate-induced structural modulation controls the photocatalytic water splitting in linkage-orientation engineered covalent organic frameworks
Palak Chugh — IIT Hyderabad

P08 A Computational Study of β-C–H Bond Activation: Variations across the three rows of Transition metals
Harsha K. Sasidharan — Indian Institute of Science, Bengaluru

P09 Free-Energy Profiling and Mechanistic Elucidation of Nucleoside Analogue-Mediated Inhibition of Viral RNA Synthesis
Blessy Elsa Joseph — University of Calicut

Poster Session II

Saturday, 5 December 2026 | 15:30–17:00 IST

SESSION CHAIR | **Susmita De, University of Calicut**

P10 Incorporating Stagnation Escape Strategies into the Bonobo Optimizer for Atomic Cluster Global Optimization
Bhrigu Chakraborty — IIT Kharagpur

P11 Bonding Insights into Metavalent Materials for Next-generation Memory
Mithu Kumari — IISER Mohali

P12 Revealing the Singlet Oxygen Reactivity in Photoredox Cyclopropanation of Unactivated Alkenes with Active Methylene Compounds
Balineni Prasad — IIT Palakkad

P13 Deciphering the mechanism of chain propagation in polymerization via alkene difunctionalisation
R. S. Malavika — IIT Palakkad

P14 Manganese-Based Catalysts for Efficient CO_2 Hydrogenation and Thereby Catalyst Design
Nikhil Mondal — IIT Palakkad

P15 Overcoming the Intrinsic Ambidenticity of Enamines in SOMO Catalysis
Vishnu Suresh M. S. — IIT Palakkad

P16 Electronic Structure, Bonding and Reactivity of Stable Two-Coordinate Acyclic Silylene
Keerthana V. — NIT Calicut

P17 Dimensionality- and Halide-Driven Electronic Reorganization of Mn^{2+} Excited States in Halide Perovskites
Athira P. — IIT Hyderabad

P18 Continuum of Secondary-Primary Interactions in Antimony Complexes and Differences in the Structures in Solution and Solid State
Annabel Benny — Indian Institute of Science, Bengaluru; IISER Thiruvananthapuram

P19 Beryllium learns Kubas Chemistry: An aromatic route to dihydrogen activation
Roshan Mahadik — Indian Institute of Science, Bengaluru