



September 22–27, 2024
Prague Congress Center, Czech Republic

Session Program – Wednesday, 25 September

Room: North Hall

09:20 AM	09:50 AM	Coffee break	Forum Hall Foyer 2
Symposium G - Wednesday Morning / 09:50 AM-11:40 AM			Chair: James Kermode
09:50 AM	10:20 AM	Keynote Lecture: Non-linear Atomic Cluster Expansion and its Graph Extension for Machine-Learning Interatomic Potentials	Yury Lysogorskiy
10:20 AM	10:40 AM	Mo-Si alloys studied by atomistic computer simulations using a novel machine-learning interatomic potential: Thermodynamics and interface phenomena	Jochen Rohrer
10:40 AM	11:00 AM	CANCELLED	Alexis Front
11:00 AM	11:20 AM	Applicability of universal machine learning interatomic potentials to the simulation of steels	Sebastián Echeverri Restrepo
11:20 AM	11:40 AM	Hyperparameter Optimization for Machine Learning Potentials: Fitting Efficient Potentials for Large Scale Materials Modelling	Daniel Thomas du Toit
11:40 AM	12:40 PM	Lunch	Forum Hall Foyer 2
Symposium G - Wednesday Afternoon / 12:40 PM-02:30 PM			Chair: Jan Janssen
12:40 PM	01:00 PM	Towards material-agnostic diverse data generation for training machine-learning interatomic potentials	Aparna P. A. Subramanyam
01:00 PM	01:20 PM	Active sampling strategies for efficient MLIP dataset development	Thomas Rocke
01:20 PM	01:40 PM	Implicit differentiation for uncertainty quantification and inverse design in large-scale material simulations	Ivan Maliyov
01:40 PM	02:00 PM	Conformal Prediction for Uncertainty Propagation in Atomistic Simulations	Iain Best
02:00 PM	02:20 PM	Automated Generation of DFT Structure Sets for Transferable Machine Learning Potentials	Marvin Poul
02:30 PM	03:00 PM	Coffee break	Forum Hall Foyer 2
Symposium G - Wednesday Afternoon / 03:00 PM-04:50 PM			Chair: Thomas Hammerschmidt
03:00 PM	03:20 PM	Thermal transport in disordered carbon and silicon from machine-learning molecular dynamics	Yanzhou Wang
03:20 PM	03:40 PM	Development of an interatomic potential for silicon carbide for crystal growth and defect calculations	Celine Halkali
03:40 PM	04:00 PM	Enhance descriptor-based approaches in Material Science	Alexandre D�ezaphie
04:00 PM	04:20 PM	Machine-learning structural stability of complex intermetallic phases	Mariano Forti
04:20 PM	04:40 PM	Automated workflows to construct and validate machine-learned interatomic potentials	Jan Janssen
04:50 PM	06:50 PM	Poster Session 2	Forum Hall Foyer 3
06:50 PM	07:10 PM	Poster Award Ceremony	Chamber Hall
07:30 PM	10:00 PM	Conference Banquet	Forum Hall



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Session Program – Wednesday, 25 September

Room: Terrace 2A

09:20 AM	09:50 AM	Coffee break	Forum Hall Foyer 2
Symposium I - Wednesday Morning / 09:50 AM-11:40 AM			Chair: Marco Salvaglio
09:50 AM	10:20 AM	Keynote Lecture: Development of comprehensive grain boundary structure-property relationships using a large dataset of bicrystals	Eric Homer
10:20 AM	10:40 AM	Convolutional Recurrent Neural Networks for tackling materials dynamics at the mesoscale	Daniele Lanzoni
10:40 AM	11:00 AM	Data assimilation to infer interfacial properties for polycrystalline equiaxed dendrites using phase-field method	Shunsuke Kanki
11:00 AM	11:20 AM	Material Point Method in Focus: Bridging the gap between experiment and simulation in abrasive event analysis	Alejandra Ventura
11:20 AM	11:40 AM	Investigating high heating rate sintering with the phase-field method	Marco Seiz
11:40 AM	12:40 PM	Lunch	Forum Hall Foyer 2
Symposium I - Wednesday Afternoon / 12:40 PM-02:30 PM			Chair: Eric Homer
12:40 PM	01:00 PM	A model for Solvation in Battery Electrolytes and analysis of Electrochemical Double Layer differential capacitance	Constantin Schwetlick
01:00 PM	01:20 PM	Large-scale phase-field simulation of microstructural evolution during solid-state sintering of BaFe ₂ As ₂ superconducting material	Akimitsu Ishii
01:20 PM	01:40 PM	Quantifying the structural lubricity of twisted bilayer graphene from the mobility of interface dislocations	Md Tusher Ahmed
01:40 PM	02:00 PM	Wettability of grain boundaries by liquid metals	Thierry Auger
02:00 PM	02:20 PM	Recovery and recrystallization of deformed metal nanoparticles	Jonathan Zimmerman
02:30 PM	03:00 PM	Coffee break	Forum Hall Foyer 2
		-	-
03:00 PM	03:20 PM	-	-
03:20 PM	03:40 PM	-	-
03:40 PM	04:00 PM	-	-
04:00 PM	04:20 PM	-	-
04:20 PM	04:40 PM	-	-
04:50 PM	06:50 PM	Poster Session 2	Forum Hall Foyer 3
06:50 PM	07:10 PM	Poster Award Ceremony	Chamber Hall
07:30 PM	10:00 PM	Conference Banquet	Forum Hall



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Prague Congress Center, Czech Republic

Session Program – Wednesday, 25 September

Room: Terrace 2B

09:20 AM	09:50 AM	Coffee break	Forum Hall Foyer 2
Symposium D - Wednesday Morning / 09:50 AM-11:40 AM			Chair: Avadh Saxena
09:50 AM	10:20 AM	Keynote Lecture: Multiscale design of permanent magnets	Thomas Schrefl
10:20 AM	10:40 AM	μ ASD, a Multiscale Approach to Magnetization Dynamics	Nastaran Salehi
10:40 AM	11:00 AM	Unconventional magnetism and spin symmetries	Libor Šmejkal
11:00 AM	11:20 AM	Mechanism of magnetization reversal in magnetite nanoparticles	Roman Gröger
11:20 AM	11:40 AM	-	-
11:40 AM	12:40 PM	Lunch	Forum Hall Foyer 2
Symposium D - Wednesday Afternoon / 12:40 PM-02:30 PM			Chair: Joseph Barker
12:40 PM	01:10 PM	Keynote Lecture: Multicaloric Effects and Materials	Lluís Manosa
01:10 PM	01:30 PM	Acceleration methods applied to the thermal homogenization optimization	Timothee Devictor
01:30 PM	01:50 PM	Flexocaloric Modeling of Ferroelastic Materials	Avadh Saxena
01:50 PM	02:10 PM	Effective material properties in flexoelectric nanocomposites	Miroslav Repka
02:10 PM	02:30 PM	-	-
02:30 PM	03:00 PM	Coffee break	Forum Hall Foyer 2
Symposium D - Wednesday Afternoon / 03:00 PM-04:50 PM			Chair: Lluís Manosa
03:00 PM	03:20 PM	Optimizing inorganic halide perovskites for photovoltaic applications: Insights from theory	Antoine Gissler
03:20 PM	03:40 PM	Integrating Digital Twin Technology with Multiscale Mechanics Modelling for Enhanced Safety and Efficiency in Energy Systems	Henry Tan
03:40 PM	04:00 PM	Liquid structure in mixtures of imidazolium based ionic liquid/carbonate solvents for application in next generation lithium ion battery electrolytes: molecular dynamics simulation	Abraham Molla Wagaye
04:00 PM	04:20 PM	The influence of a non-static Potential Energy Surface on the ion-diffusivity of crystalline solids	Fabian Schwarz
04:20 PM	04:40 AM	-	-
04:50 PM	06:50 PM	Poster Session 2	Forum Hall Foyer 3
06:50 PM	07:10 PM	Poster Award Ceremony	Chamber Hall
07:30 PM	10:00 PM	Conference Banquet	Forum Hall



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Session Program – Wednesday, 25 September

Room: South Hall 2A

09:20 AM	09:50 AM	Coffee break	Forum Hall Foyer 2
Symposium N - Wednesday Morning / 09:50 AM-11:40 AM			Chair: Shigenobu Ogata
09:50 AM	10:20 AM	Keynote Lecture: Mechanics of extremely heterogeneous materials	Ting Zhu
10:20 AM	10:40 AM	Machine Learned Interatomic Potential for Atomic Simulation of Dislocation Plasticity in Ceramics	Shihao Zhang
10:40 AM	11:00 AM	Connecting dislocation shape and local stresses with machine learning	Dénes Berta
11:00 AM	11:20 AM	-	-
11:20 AM	11:40 AM	-	-
11:40 AM	12:40 PM	Lunch	Forum Hall Foyer 2
Symposium N - Wednesday Afternoon / 12:40 PM-02:30 PM			Chair: Penghui Cao
12:40 PM	01:10 PM	Keynote Lecture: Phase stability and radiation effects in high-entropy ceramics	Izabela Szlufarska
01:10 PM	01:40 PM	Keynote Lecture: The role of atomic-scale defects in the strength of refractory complex concentrated alloys at high temperature	Jaime Marian
01:40 PM	02:00 PM	Revisiting the vacancy diffusion behavior under the influence of solute trapping in dilute alloys	Xue-Zhou Wang
2:00 PM	2:20 PM	-	-
02:30 PM	03:00 PM	Coffee break	Forum Hall Foyer 2
Symposium N - Wednesday Afternoon / 03:00 PM-04:50 PM			Chair: Jaime Marian
03:00 PM	03:30 PM	Keynote Lecture: Simulation-informed models for amorphous metal mechanical property prediction	Michael Falk
03:30 PM	03:50 PM	Graph Neural Networks as a Gateway to New Possibilities in Metallic Glass Property Prediction and Design	Qi Wang
03:50 PM	04:10 PM	Insight Beyond Short-Range Order in Metallic Glasses Revealed by Machine Learning	Yue Fan
04:10 PM	04:30 PM	Development and application of machine learning interatomic potentials to the investigation of metallic glasses from the Zr-Cu-Al system	Antoni Wadowski
04:30 PM	04:50 PM	Microstructure Modeling and Analysis in Complex Materials	Pejman Tahmasebi
04:50 PM	06:50 PM	Poster Session 2	Forum Hall Foyer 3
06:50 PM	07:10 PM	Poster Award Ceremony	Chamber Hall
07:30 PM	10:00 PM	Conference Banquet	Forum Hall



September 22–27, 2024
Prague Congress Center, Czech Republic

Session Program – Wednesday, 25 September

Room: South Hall 2B

09:20 AM	09:50 AM	Coffee break	Forum Hall Foyer 2
Symposium A - Wednesday Morning / 09:50 AM-11:40 AM			Chair: Caroline Traisnel
09:50 AM	10:20 AM	Keynote Lecture: Quantum mechanical based modelling of electrified solid/liquid interfaces – the example of corroding Mg	Mira Todorova
10:20 AM	10:40 AM	Design criteria for zero-strain cathode materials of the tungsten bronze type compounds A_xFeF_3 (A=Li, Na, K) by first-principles	Aljoscha Felix Baumann
10:40 AM	11:00 AM	QM/MM simulations of the electrochemical interface	Pablo Ordejon
11:00 AM	11:20 AM	Multi-scale Modeling of Thin Film Deposition for Metal Anode batteries	Musanna Galib
11:20 AM	11:40 AM	Molecular Modelling of Dynamics and NMR Properties in Lithium Solid-State Electrolytes for Li-ion Solid Batteries	Mahmoud Attia
11:40 AM	12:40 PM	Lunch	Forum Hall Foyer 2
Symposium A - Wednesday Afternoon / 12:40 PM-02:30 PM			Chair: Mira Todorova
12:40 PM	01:00 PM	Unraveling the electrochemical behavior of ferrous alloys: A first-principles study	Pragyandipta Mishra
01:00 PM	01:20 PM	Segregation and diffusion of H atoms and defects formation at the W/Cu interface	Yves Ferro
01:20 PM	01:50 PM	Keynote Lecture: First-principles study of charged point defects properties in forsterite	Caroline Traisnel
01:50 PM	02:10 PM	Ultimate mechanical properties of $(Mg,Fe)_2SiO_4$ olivine: fayalite vs. forsterite	Karine Gouriet
02:10 PM	02:30 PM	First-principles study of complex ferrimagnetic states in maghemite-related nanoparticles	Valentina Berecová
02:30 PM	03:00 PM	Coffee break	Forum Hall Foyer 2
Symposium A - Wednesday Afternoon / 03:00 PM-04:50 PM			Chair: Celine Varvenne
03:00 PM	03:30 PM	Keynote Lecture: Pathways for the preparation of functional coatings by simulations at various scales	Jiri Houska
03:30 PM	03:50 PM	Atomistic investigations of doping in SiC polytypes	Zahra Rajabzadeh
03:50 PM	04:20 PM	Keynote Lecture: Trapping and mobility properties of impurities in actinide oxides: a DFT+U study	Mathieu Gascoin
04:20 PM	04:40 PM	Point Defects in Oxides Promote Molecular Transformation through Interfacial Charge Transfer	Bin Wang
04:50 PM	06:50 PM	Poster Session 2	Forum Hall Foyer 3
06:50 PM	07:10 PM	Poster Award Ceremony	Chamber Hall
07:30 PM	10:00 PM	Conference Banquet	Forum Hall



September 22–27, 2024
Prague Congress Center, Czech Republic

Session Program – Wednesday, 25 September

Room: South Hall 3A

09:20 AM	09:50 AM	Coffee break	Forum Hall Foyer 2
Symposium E - Wednesday Morning / 09:50 AM-11:40 AM			Chair: Anter El-Azab
09:50 AM	10:20 AM	Keynote Lecture: Dislocation microplasticity in irradiated and inhomogeneous alloys	Anter El-Azab
10:20 AM	10:40 AM	Non-classical Critical Void Nuclei From a Vacancy-Based Phase-Field Model	Kevin Pendl
10:40 AM	11:00 AM	Hyperthermal erosion of thermal protection materials under LEO and sub LEO environment : Reactive molecular dynamic simulation	Inseok Jeon
11:00 AM	11:20 AM	High dose irradiation of tungsten with realistic dose rate and atomistic resolution	Jintong Wu
11:20 AM	11:40 AM	-	-
11:40 AM	12:40 PM	Lunch	Forum Hall Foyer 2
Symposium E - Wednesday Afternoon / 12:40 PM-02:30 PM			Chair: Fei Gao
12:40 PM	01:10 PM	Keynote Lecture: Defect Accumulation of Radiation Damage in Metals: Challenges and Case Study	Fei Gao
01:10 PM	01:30 PM	Fast low-temperature irradiation creep driven by athermal defect dynamics	Max Boleininger
01:30 PM	01:50 PM	Microstructure Evolution in Irradiated Tungsten with Helium implantation	Pengchuang Liu
01:50 PM	02:10 PM	Dislocation climb driven by lattice diffusion and core diffusion	Fengxian Liu
02:10 PM	02:30 PM	Techniques for large-scale high-dose simulations of single- and polycrystalline tungsten	Fredric Granberg
02:30 PM	03:00 PM	Coffee break	Forum Hall Foyer 2
Symposium E - Wednesday Afternoon / 03:00 PM-04:50 PM			Chair: Jing Zhang
03:00 PM	03:30 PM	Keynote Lecture: Multi-scale modeling of the fission gaseous swelling and release coupling behaviors of nuclear fuels	Jing Zhang
03:30 PM	03:50 PM	Multiscale Modelling of nuclear oxide fuel behaviour: from atomic scale simulations to fuel performance codes	Emeric Bourasseau
03:50 PM	04:10 PM	Multi-scale modeling of the creep-related multi-fields during the uniaxial tests for crystalline UO ₂ under irradiation and high temperature conditions	Xie Zhexiao
04:10 PM	04:30 PM	Simulations of MOX fuel under irradiation: Linking microstructure and mechanical properties	Laurent Van Brutzel
04:30 PM	04:50 PM	-	-
04:50 PM	06:50 PM	Poster Session 2	Forum Hall Foyer 3
06:50 PM	07:10 PM	Poster Award Ceremony	Chamber Hall
07:30 PM	10:00 PM	Conference Banquet	Forum Hall



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Prague Congress Center, Czech Republic

Session Program – Wednesday, 25 September

Room: South Hall 3B

09:20 AM	09:50 AM	Coffee break	Forum Hall Foyer 2
Symposium B - Wednesday Morning / 09:50 AM-11:40 AM			Chair: Yinan Cui
09:50 AM	10:20 AM	Multiscale Modelling of High Strain Rate Plastic Deformation in Tantalum	Dan Mordehai
10:20 AM	10:40 AM	Modeling Intrinsic Uncertainty from Material Microstructure Sources at the Engineering Scale using Bayesian Symbolic Regression	Jacob Hochhalter
10:40 AM	11:00 AM	Initializing grain and sub-grain scale residual stress in crystal plasticity simulations	Michael Sangid
11:00 AM	11:20 AM	Simulation of static recrystallization in A1100 aluminum alloy using Bayesian data assimilation of multi-phase-field method and in-situ observation	Motoki Umezawa
11:20 AM	11:40 AM	Analysis and modelization of the internal and effective stresses in cyclic plastic straining	Jaroslav Polák
11:40 AM	12:40 PM	Lunch	Forum Hall Foyer 2
Symposium F - Wednesday Afternoon / 12:40 PM-02:30 PM			Chair: Carl Goodrich
12:40 PM	01:10 PM	Keynote Lecture: Coarse-grained hydrodynamic simulations of active and driven particles in complex fluids	Andreas Zöttl
01:10 PM	01:30 PM	Understanding nanoparticle transport through hydrogels under acoustic streaming with molecular simulations	Pablo M. Blanco
01:30 PM	01:50 PM	CANCELLED	Arnab Chanda
01:50 PM	02:20 PM	Keynote Lecture: Modeling charged polymers for soft materials design	Andrea Giuntoli
02:20 PM	02:30 PM	-	-
02:30 PM	03:00 PM	Coffee break	Forum Hall Foyer 2
-	-	-	-
03:00 PM	03:30 PM	-	-
03:30 PM	03:50 PM	-	-
03:50 PM	04:10 PM	-	-
04:10 PM	04:30 PM	-	-
04:30 PM	04:50 PM	-	-
04:50 PM	06:50 PM	Poster Session 2	Forum Hall Foyer 3
06:50 PM	07:10 PM	Poster Award Ceremony	Chamber Hall
07:30 PM	10:00 PM	Conference Banquet	Forum Hall



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Session Program – Wednesday, 25 September

Room: South Hall 3C

09:20 AM	09:50 AM	Coffee break	Forum Hall Foyer 2
Symposium C - Wednesday Morning / 09:50 AM-11:40 AM			Chair: Jan Fikar
09:50 AM	10:20 AM	Keynote Lecture: The Origin of photoplasticity in II-VI semiconductors	Maryam Ghazisaeidi
10:20 AM	10:40 AM	Dislocations in SrTiO ₃ perovskite: neutral vs charged, glide vs climb	Pierre Hirel
10:40 AM	11:00 AM	Dislocation mobility and cross-slip processes of the screw dislocation in UO ₂	Jules-Elemir Suchorski
11:00 AM	11:20 AM	The Influence of Helium on Screw Dislocation Mobility in Tungsten	Matt Nutter
11:20 AM	11:40 AM	Impact of hydrogen on screw dislocation glide in tungsten	Thomas leveau
11:40 AM	12:40 PM	Lunch	Forum Hall Foyer 2
Symposium C - Wednesday Afternoon / 12:40 PM-02:30 PM			Chair: Maryam Ghazisaeidi
12:40 PM	01:10 PM	CANCELLED	Nicolas Bertin
01:10 PM	01:30 PM	Compressing and forecasting atomic simulations of plasticity with descriptors	Thomas Swinburne
01:30 PM	01:50 PM	Identification of dislocation structures in experimental Laue microdiffraction patterns	Benjamin Udofia
01:50 PM	02:10 PM	Hybrid QM/ML study of carbon induced screw dislocation pinning in tungsten	Petr Grigorev
02:10 PM	02:30 PM	Study of the Interaction between hydrogen and screw dislocations in Alpha-Fe by multi-scale simulations	Margot Lucas
02:30 PM	03:00 PM	Coffee break	Forum Hall Foyer 2
Symposium C - Wednesday Afternoon / 03:00 PM-04:50 PM			Chair: Giacomo Po
03:00 PM	03:30 PM	Keynote Lecture: Cross-scale covariance for material property prediction	Vasily Bulatov
03:30 PM	03:50 PM	Unbiased Atomistic Predictions of Crystal Dislocation Dynamics using Bayesian Force Fields	Amir Naghdi
03:50 PM	04:10 PM	Universal algorithm for ab initio-accurate atomistic simulations of dislocations	Max Hodapp
04:10 PM	04:30 PM	Developing Extended Modified Embedded-Atom Method Potentials for Atomistic Modelling on Plastic Deformation of BCC Transition Metals	Rui Wang
04:30 PM	04:50 PM	Edge dislocation dynamics in Ni-based superalloys from atomistic simulations: parameterisation and uncertainty quantification	Peter Brommer
04:50 PM	06:50 PM	Poster Session 2	Forum Hall Foyer 3
06:50 PM	07:10 PM	Poster Award Ceremony	Chamber Hall
07:30 PM	10:00 PM	Conference Banquet	Forum Hall



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Session Program – Wednesday, 25 September

Room: Chamber Hall

09:20 AM	09:50 AM	Coffee break	Forum Hall Foyer 2
Symposium O - Wednesday Morning / 09:50 AM-11:40 AM			Chair: Manas Upadhyay
09:50 AM	10:20 AM	Keynote Lecture: Fast model of directed energy deposition from thermal analysis to microstructure, and part-scale residual stress estimation	Daniel Weisz-Patrault
10:20 AM	10:40 AM	Influence of laser profiles on melt pool dimensions for LPBF processes analyzed by thermal simulation	Raveeshankar Sambathkumar
10:40 AM	11:00 AM	A Microstructure Modelling Framework for Multi-Laser Powder Bed Fusion of Ti-6Al-4V	Hugh Banes
11:00 AM	11:20 AM	Leveraging laser parameters and layer remelting to tailor microstructure in laser powder bed fusion	Nicole Aragon
11:20 AM	11:40 AM	-	-
11:40 AM	12:40 PM	Lunch	Forum Hall Foyer 2
Symposium O - Wednesday Afternoon / 12:40 PM-02:30 PM			Chair: Damien Tournet
12:40 PM	01:10 PM	Keynote Lecture: Machine learning for next generation additively manufactured structural alloys in extreme environments	Benjamin Glaser
01:10 PM	01:30 PM	Microstructure-informed modeling of additively manufactured 316L stainless steel aortic stents	Yu Qiao
01:30 PM	01:50 PM	Numerical investigations of melt pool and grain growth in metal additive manufacturing process	Raveeshankar Sambathkumar
01:50 PM	02:10 PM	Multi-scale modeling study of gamma prime formation in Ni based superalloys during electron beam additive manufacturing	Rajeev Ahluwalia
02:10 PM	02:30 PM	Multi-phase-field method-based multiscale and multiphysics modeling and high-performance computing of metal additive manufacturing	Tomohiro Takaki
02:30 PM	03:00 PM	Coffee break	Forum Hall Foyer 2
Symposium O - Wednesday Afternoon / 03:00 PM-04:50 PM			Chair: Allison Beese
03:00 PM	03:30 PM	Keynote Lecture: Multi-scale multi-physics modelling of heterogeneous non-equilibrium microstructure in metal additive manufacturing	Chinnapat Panwisawas
03:30 PM	03:50 PM	Phasefield modelling of solidification pores during additive manufacturing of a nickel-based superalloy	Mostafa Salem
03:50 PM	04:10 PM	Atomic and microstructural simulations of rapid solidification refractory alloys	Joni Kaipainen
04:10 PM	04:30 PM	Multiscale analysis of rapid solidification in additive manufacturing via quantitative simulations and in-situ monitoring	Tatu Pinomaa
04:30 PM	04:50 PM	Multiscale modeling of rapid solidification in laser powder-bed fusion of a Magnesium alloy	Damien Tournet
04:50 PM	06:50 PM	Poster Session 2	Forum Hall Foyer 3
06:50 PM	07:10 PM	Poster Award Ceremony	Chamber Hall
07:30 PM	10:00 PM	Conference Banquet	Forum Hall