

The 10th ICReDD International Symposium POSTER SESSION

PRESENTERS, POSTER NUMBERS AND POSTER TITLES

October 8th, 2026

PRESENTER	No.	TITLE
Umair UMER	1	Stabilizing High-Order Phase-Space Dynamics: A Diagnostic Chebyshev Framework
Pinku NATH	2	ChemOntology: An xTB-to-DFT Transformation Workflow for Reaction-Path Search
Ryuto KAMBARA	3	Floquet-Based Molecular Dynamics on Laser-Induced Potential Energy Surfaces
Tetsuya YAMAMOTO	4	Kinetic theory of mechanochemical reaction
Jieun JUNG	5	Versatile (PNNP)Ir Catalysts for Sustainable CO ₂ Utilization
Gumi WEI	6	Force-Driven Growth and Fibrillogenesis Create Anisotropic Flaw-Resistant Hydrogels
Saswati ADHIKARY	7	Near-Infrared Photoimmunotherapy: Development of Novel Anticancer Agents
Yuhua SUN	8	Synthesis and Spectroscopic Property of α — β linked Cyclo[4]pyrrole
Yoshiki KAWARA	9	Synthetic Studies toward Unified Total Synthesis of Indolizidine Alkaloids
Hongguang LIAO	10	Ionic Screening-Tolerant Polyelectrolyte Hydrogels via Bioinspired Adjacent Charged—Aromatic Sequences
Taise NAKAJIMA	11	Development of organic X-ray scintillator using crystalline gear-shaped Au(I) complex with two-dimensional porous structure
Trond LINJORDET	12	Towards Task-Appropriate Validation of Generated Molecular Geometries
Hiroki IWAI	13	Bayesian Optimization of Adsorption Structures Using the Tree-structured Parzen Estimator and First-Principles Calculations
Kaveri PRASAD	14	A Global Multi-Solvent Machine Learning Framework for Predicting Azo Photoswitch Kinetics and Spectra
Sagar GHORAI	15	Toward Reaction Vessel Mimicry: Machine Learning Assisted Automated Exploration of Alkene Polymerization and CO Coupling Reactions

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PRESENTER	No.	TITLE
Narendra Nath PATI	16	Synthesis of Calix[4]thiazole and Structural Characterization of Its Metal Complexes
Mini Bharati AHIRWAR	17	Theoretical Insights into Rhodium-Catalyzed Kumada—Tamao—Corriu Coupling: Critical Roles of a Pincer-Type Alumanyl Ligand
Ryota SHIJO	18	Carbonyl-selective Allylation of 1,3-Diketones Enabled by Light and Pt Catalyst
Takuto KOYAMA	19	Structure Exploration of Spinel High-Entropy Oxides Incorporating Configurational Entropy
Masaya ENDO	20	Visible-Light-Induced Boron-Catalyzed Alkyne-de Mayo Reaction
Reo KURIHARA	21	Bayesian Molecular Optimization of Rapid Spin-Conversion Materials for Efficient Organic Light-Emitting Diodes
Wongsathorn KAEWRAUNG	22	Revealing the Origin of γ -Selectivity in Cross-Coupling Through NNP/AFIR-Based Reaction Path Exploration
Hirokazu AKADA	23	Effect of Exchange-Correlation Functionals on the Evaluation of the Absolute Potential of the Standard Hydrogen Electrode
Keishi KAWAZU	24	Energy Decomposition Analysis of Alkane and Aldehyde Adsorption on ZnO and MgO Surfaces
Masamichi IMAJO	25	A synthetic hydrogel scaffold inducing stem cell signatures in colorectal cancer cells
Rikito HASUO	26	Reaction Design for Photocatalytic Carboxylation of Aniline Derivatives with CO ₂
Xingyu TANG	27	Transferability for Reaction Path Search: From Small to Large
Jinyao XU	28	Heptazine—Carboline-Based an Inverted Singlet—Triplet Material for High-Efficiency Organic Light-Emitting Diodes
Yoshichika TSUBAKIHARA	29	Construction of Crystalline Toroidal Mesoscale Intermolecular Hexa-Gear Structures Composed of Triptycene Derivatives
Kosei TAKAHASHI	30	Synthetic Study of Momilactone B

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Ryo KURAHASHI	31	From Phase-Space Dynamics to Molecular Motion: Interpreting Nonreactive-Mode Effects on Saddle Passage in HCN
Kai OSHIRO	32	Constructing Machine-Learning Force Fields for Oxygen Vacancy on CeO ₂ Surfaces
Simon COOPER	33	Intramolecular Hydride Transfer Racemization Coupled with Enzymatic Kinetic Resolution Enables Asymmetric Syntheses of Caged Compounds
Itsuki KONDO	34	Theoretical Study on the C(sp ₃)—P Bond Cleavage Mechanism in the Photocatalytic Dealkylation of Tertiary Phosphines
Yuji NAITOH	35	Methane combustion mechanism generation using AFIR method and kinetic simulation
Ruben STAUB	36	NNP-AFIR Accelerated Reaction Path Search: Solving the Passerini Mechanism Controversy
Yusuke SHIRAI	37	Perivascular Microenvironment of Glioblastoma Stem Cells and Heparan Sulfate Proteoglycans