

The 9th ICReDD International Symposium POSTER SESSION

PRESENTERS, POSTER NUMBERS AND POSTER TITLES

October 17th, 2025

PRESENTER	No.	TITLE
Min GAO	1	Structure Re-programming by Systematic Exploration of Molecular Structures
Yongjie SHEN	2	Theoretical Understanding and Design of Single-Atom and Dual-Atom Active Sites on Oxide Surfaces
Wongsathorn KAEWRAUNG	3	Computational Screening for Single Metal Atom Catalysts on Mo ₂ B ₂ O ₇ Support as Cathode Materials of Li-S Batteries
Godfrey KALANZI	4	Sustainable Catalytic Strategies for Precision Bond Formation: Bridging Molecular Design and Functional Materials
Younis RASOOL	5	Skeletal Editing via CH→N Atom Swapping in Fused Pyridines: Access to Triazolo[5,1-a]isoquinoline, Triazolo[1,5-a]quinoline and Triazolo-[1,5-a]pyridines Frameworks
Kai OSHIRO	6	Constructing Machine-Learning Force Fields for Oxygen Vacancy on CeO ₂ Surfaces
Saswati ADHIKARY	7	Development of New Photoimmunotherapeutic (PIT) Anti-cancer Drugs with Potential Synergy Anti-angiogenic Effect
Kaveri PRASAD	8	Predictive Modeling and Experimental Validation of azo-photoswitches in Diverse Solvents
Ganesh PATIL	9	Metal Oxide with its DFT Study
Shih-Ching CHUANG	10	Pd(II)-Catalyzed C(sp ²)-H Alkenylation of 2-Amino Biaryls with Bulky Internal Alkynes: From Alkenylation to Orthogonal Polycyclic Hydrocarbons
Sagar GHORAI	11	Machine Learning Unlocks Automated s-block Reaction Network Exploration: Integration of 2 to 6 CO Coupling by [Mg(I)] Complexes
Yuki IDE	12	Inkjet Printing-Assisted Image Machine Learning System for Chemical Analysis
Tsuyoshi MITA	13	β-Amino Acid Synthesis from CO ₂
Pinku NATH	14	CHEMONT: Leveraging Chemical Knowledge for Smarter Reaction Network Exploration
Balasubramaniyan SAKTHIVEL	15	Automated Synthesis and Fragment Descriptor-Based Machine Learning for Retention Time Prediction in Supercritical Fluid Chromatography

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PRESENTER	No.	TITLE
Vitor ALCANTARA FERNANDES	16	A Comprehensive Optimization for Asymmetric Catalysis
Yuqing ZHENG	17	Reductive aza-Pauson-Khand Reaction
Satoshi MATSUTANI	18	Developing a Conformational Sampling Method for Transition State Structures with Varying Reaction Centers
Pei-Zhen XIE	19	Synergy between Pd-NAPA Precatalyst and Mechanochemistry for Green Catalysis
Shreya M J	20	Synthesis and Development of Shortwave-infrared (SWIR)-emitting Cyanine Dyes for In Vivo Imaging
SAID BYADI	21	Photoswitchable Wnt Pathway Agonists: Molecular Docking and Dynamics Reveal Selective Binding of cis-Isomer to Frizzled Receptors
Risa AMANO	22	Optical Force and Torque on C ₃ H ₆ Molecule: A Real-time Real-space TDDFT Study
Ryuto KAMBARA	23	The Reaction Path Network and Pathways Hidden by Dynamical Effects
Masamichi IMAJO	24	Application of Synthetic Hydrogel Technologies to Cancer Research
Haixin ZHANG	25	Organocatalyst-Loaded Double-Network Gels for High-Performance Catalytic Reactions
Shunsuke OKADA	26	Development and Catalytic Performance of a Spirocyclic Borate as an Anionic Photosensitizer
Koki OGAWARA	27	Rational Design of Caged Compounds via X-Ray-Induced Azo Bond Cleavage
Jan SAMSONOWICZ-GÓRSKI	28	Catalytic Asymmetric Diels-Alder Reactions of Acyclic Disubstituted Enones with Hydrocarbon Dienes
Mengfei WANG	29	Lanthanide Luminescence in Sensing
Feixue LU	30	Fracture-triggered Templated Polymerization for Real-time Self-reinforcement of DN Gels without Mechanophores

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SHUN ZHOU	31	Photocatalytic Radical Trifluoromethylation Using Fluoroform
Ken HIROSE	32	Development of Virtual Borane: Expansion of Virtual Ligand Method for the Design of Triarylborane Catalysts
Amitabha DAS	33	Single and Dual Atom Alloy Catalysts for the CO ₂ Reduction Reactions
Takuma NAKAI	34	Dynamic Molecular Triplet Excitons Tune Lanthanide Emission Lifetime
Nakaba AKUTSU	35	Triarylphosphine Sulfides as a Hydrogen Atom Abstraction Catalyst under Photoredox Conditions: Reactivity, Scope, and Regioselectivity
Ruben STAUB	36	NNP-AFIR Accelerated Reaction Path Search: Solving the Passerini Mechanism Controversy
Kaoru KOIZUMI	37	Circularly Polarized Luminescence from Transparent Films Composed of Chiral Tetrakis-type Eu(III) Complexes
Farkas DOMAHIDY	38	Triarylpyrylium-based DNA-binding Dyes - Synthesis and Fluorescence Properties
Ali HAIDER	39	Tangled Threads: Multiscale Mapping of Collagen Entanglement and Supramolecular Chirality in Human Skin
Tetsuya YAMAMOTO	40	Crossover of Limiting Processes of Mechanochemical Reaction by Ball-milling
Itsuki KONDO	41	A Systematic Exploration of Nonradiative Decay Paths in Carbohelicenes: Contribution of the Cyclization Mechanism
Tatsuhiro NAKANISHI	42	Analyzing Mechanisms of Post-transition State Bifurcation through Natural Reaction Orbitals
Fengshi QI	43	Synthesis of an N-Doped Nanographene Containing 1,12-Diazatriphenylene Scaffold by Cyclodehydrogenation Reaction
Joel MUYOMBA	44	Surface-associated N-Terminal Immobilization Strategy to Enhance Hydrolysis Activity of Cutinase Toward Polyethylene Terephthalate Film.
Gloria KAMWEZI	45	Development of Eco-Friendly Bioplastic from Chitin, Chitosan and PCL Blends