

6th ICReDD INTERNATIONAL SYMPOSIUM POSTER SESSION

PRESENTERS, POSTER NUMBERS AND POSTER TITLES

September 10th, 2023

PRESENTER	No.	TITLE
Yuki Ide	1	Application of Machine Learning System Based on Solid State Images for Chemical Research
Tasuku Nakajima	2	Swelling-induced Strand Scission of a Polymer Network
Mengfei Wang	3	Water-soluble Eu(III) complex for Human brain tumor diagnosis
Masamichi Imajo	4	Application of synthetic hydrogel technology to the control of cancer and pluripotent stem cells
Tsuyoshi Mita	5	Automated Reaction-Path Search for Stereospecific Pericyclic Reactions by Quantum-Chemistry-Aided Retrosynthetic Analysis Using the AFIR Method
Yoshito Heike	6	Phosphine-Catalyzed sp^3 -C-H Amination of 2-Alkylpyridines
Soichiro Mori	7	Design of Acridinium Amidate as The Catalyst for Photoinduced Direct Hydrogen Atom Transfer
Takuma Ito	8	Kinetic Analysis of Chemical reactions including dynamical bifurcations by combining reaction path network and machine learning
Shinnosuke Sunazaki	9	Analysis of reaction path networks considering stereo configurations: An application to pericyclic reactions
Pavel Sidorov	10	Fragment descriptors for prediction of enantioselectivity in asymmetric catalysis
Seonghwan Kim	11	Diffusion-based Generative AI for Exploring Transition States from 2D Molecular Graphs
Jun Hyeong Kim	12	Discovery of Thermally Activated Delayed Fluorescence Materials Using the Deep Generative Model
Jeheon Woo, Seonghwan Kim, Sunghwan Choi, and Woo Youn Kim	13	Development of GPU-Accelerated Real-Space Density Functional Theory Code
Priya Saha	14	Construction of Functionalized Red-Light Photoswitches by Selective Copper-Catalyzed Indigo N-Arylation

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Saeesh R. Mangaonkar	15	γ -Lactone Synthesis from Allylic Alcohols Using the CO ₂ Radical Anion
Anna Nožičková	16	Photocatalysis and photoswitching of covalently dynamic systems
Akihiro Mutsuji	17	Evaluation of electron self-exchange rate constants of transition metal complexes by crossing point optimization using an energy extrapolation method
Keisuke Kondo	18	Mechanochemistry Enabling Highly Efficient and Air-Tolerant Birch Reduction With Sodium Lumps
Ryota Isshiki	19	Reductive Coupling Reaction between Aryl Bromides and Alkyl Pyridinium Salts Using Solid-state Photoredox Reaction
Xihong Wang	20	General Synthesis of Novel Chiral Silyl Transfer Reagents: Silicon-Stereogenic Optically Active Silylboranes and Their Application
Kai Sun	21	Data-Assisted Development of Boron Catalysis for Functionalization of Free Carboxylic Acids
G. Krishnan Chandu	22	A Theory-Driven Radical Functionalization of Small Ring Compounds to Synthesize Unsymmetric Diphosphine Ligands
Philippe Gantzer	23	Representation of Reaction Networks by Generative Topographic Mapping
Mikhail Tsitsvero, Mingoo Jin, Andrey Lyalin	24	Thermodynamics of molecular gears in solid state by machine learning
Junpei Shimosato	25	Photoinduced Platinum-catalyzed Allylation of α -Diketones with Allylic Carbonates
Ruben Staub	26	Accelerating Artificial Force Induced Reaction path search with Neural Network Potentials
Marina Mizuno	27	Development of Circularly Polarized Luminescent Materials with Chiral Binaphthyl Structures through Theoretical Calculations of Their Excited States
Bastian Bjerkem Skjelstad	28	A Computational Study on the Early-Stage Self-Assembly of the SIFSIX-3-Zn Metal-Organic Framework

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Dennis Chung-Yang Huang	29	Red-Light Photoswitching of Indigos in Polymer Thin Films
Hikaru Yamamoto	30	Two-dimensionally geared intermolecular structure in a crystal formed by Au(I) complexes with triptycene and triadamantylphosphine
Kenichiro Saita	31	The Conrotatory and Disrotatory Ring-Opening Reaction Pathways of 1,3-Cyclohexadiene
Nobuya Tsuji, Pavel Sidorov, Chendan Zhu, Yuuya Nagata, Timur Gimadiev, Alexandre Varnek, Benjamin List	32	Predicting Highly Enantioselective Catalysts Using Tunable Fragment Descriptors
Tomislav Rozic	33	Insights into non-statistical chemical reactivity from a vibrational relaxation model
Hitoshi Nabata	34	Systematic Reaction Path Search on an Oxide Surface: A Case Study on Complete Oxidation of Methane on the PdO (101) Surface
Seiji Akiyama, Yu Harabuchi, Satoshi Maeda, Yuuya Nagata	35	Insertion of a Boron Atom into a Benzene Ring: Reactions, Mechanism, and DFT calculations
Amit K Jaiswal	36	Selective Single Hydrodefluorination of Trifluoromethyl Arenes with NHC-Boranes via Organophotoredox Catalysis
Yuuya Nagata	37	<i>In Silico</i> Analysis for the Modification of the Reactants: Tetraborylation of <i>p</i> -Benzynes Generated by the Masamune-Bergman Cyclization
Yuriko Ono, Kiyoshi Yagi, Toshiyuki Takayanagi, Tetsuya Taketsugu	38	Anharmonic vibrational state computations to reveal the disappearance mechanism of the fundamental peak of noble gas complex