	POSTER SESSION III
	Tuesday 23/09/2025
1	Nikolaos Pliatsios LUMINESCENT METAL-ORGANIC FRAMEWORKS AS AN EFFECTIVE ALTERNATIVE FOR HEAVY METAL DETECTION IN AQUEOUS ENVIRONMENT
2	Laiyu Zhang BOOSTING ONE-STEP PROPYLENE PURIFICATION VIA HYDROGEN BONDED FRAMEWORKS WITH OPEN PYRENE SITE
3	Megan O'Shaughnessy STABLE TRIPTYCENE HALIDE SALTS WITH HIGH POROSITY
4	Avanti Chakraborty ENHANCING PHOTOCATALYTIC HYDROGEN PEROXIDE GENERATION BY TUNING HYDRAZONE LINKAGE DENSITY IN COVALENT ORGANIC FRAMEWORKS
5	Rishabh Dubey METAL-ORGANIC FRAMEWORK-BASED GREEN POROUS LIQUID FOR ATMOSPHERIC ${\rm CO}_2$ CAPTURE & CONVERSION
6	Dipanjan Majumder NANO-SPRINGE ENRICHED HIERARCHICAL POROUS MOP/COF HYBRID AEROGEL: EFFICIENT RECOVERY OF GOLD FROM ELECTRONIC WASTE
7	Joana Araújo COVALENT ORGANIC FRAMEWORKS MEMBRANES FOR PHARMACEUTICALS' EXTRACTION FROM WATERS
8	Shaghayegh Naghdi OVERCOMING DIFFUSION AND STABILITY LIMITATIONS IN METAL-ORGANIC FRAMEWORKS FOR WATER PURIFICATION
9	Arjun Warrier DISORDER DRIVEN TRIPHENYLAMINE BASED MONOLITHIC COVALENT ORGANIC FRAMEWORK FOR THE EFFICIENT REMOVAL OF TOXIC OXO-ANIONS FROM WATER
10	Bing Wang OPTIMIZING THE PIEZOCATALYTIC HYDROGEN PRODUCTION ACTIVITY OF METAL-ORGANIC FRAMEWORKS THROUGH PRECISE DEFECT ENGINEERING
11	Damian Makowski PHOTOCATALYTIC ACTIVITY OF COF-BASED MATERIALS MODIFIED WITH CUS QUANTUM DOTS: INFLUENCE OF MONOMER TYPE AND MODIFIER CONTENT
12	Hongryeol Yun THE FIRST POST-SYNTHETIC MODIFICATION STRATEGY OF VINYLENE-LINKED COVALENT ORGANIC FRAMEWORK FOR BOOSTING PHOTOCATALYTIC PERFORMANCE
13	Soumya Kanti Mondal CLUSTER METALATION AND POST-SYNTHETIC PORE MODIFICATION OF MOF-808 TOWARDS PHOTOCATALYTIC CO_2 REDUCTION TO ETHANOL
14	Nada Elmerhi TUNING CORE FLEXIBILITY AND CURVATURE IN AZINE-LINKED COVALENT ORGANIC FRAMEWORKS FOR ULTRASENSITIVE IMPEDITIVE SENSING OF GLUCOSE
15	Mehdi Ghasemi COMPUTATIONAL INSIGHTS INTO ADVANCED DESIGN OF MIXED MATRIX MEMBRANES FOR GAS SEPARATION

16	Michail Vlachos MULTISCALE COMPUTATIONAL INSIGHTS INTO THE PFOA ADSORPTION BY CHEMICALLY ENGINEERED MOF-808
17	Mihails Arhangelskis TOPOLOGICAL AND STRUCTURAL DIVERSITY OF ZEOLITIC IMIDAZOLATE FRAMEWORKS EXPLORED THROUGH CRYSTAL STRUCTURE PREDICTION
18	Antonios Sarikas GAS ADSORPTION MEETS DEEP LEARNING
19	Bramantya Bramantya MACHINE LEARNING POTENTIALS FOR CRYSTAL STRUCTURE PREDICTION OF MAGNETIC METAL-ORGANIC FRAMEWORKS
20	Catherine Mollart HOW DOES INTERLAYER SPACING INFLUENCE COVALENT ORGANIC FRAMEWORK BAND GAPS?
21	Charalampos Livas MOFSYNTH: A COMPUTATIONAL TOOL TOWARD SYNTHETIC LIKELIHOOD PREDICTIONS OF MOFS
22	Charl Bezuidenhout DYNAMIC SYNERGY: PROBING MULTI-ELEMENT MOTION IN FLEXIBLE MOFS WITH COMPUTATIONAL MODELLING AND SOLID-STATE NMR
23	Chi Cheng (Cecilia) Hong TOWARDS GREENER REFRIGERANTS: SIMULATING ADSORPTION REFRIGERATION IN MOFS AND THE ROLE OF CORRELATED DISORDER
24	Dinga Wonanke INSIGHTS INTO THE ELECTROCHEMICAL PROPERTIES OF METAL-ORGANIC FRAMEWORKS FOR APPLICATIONS IN DIVERSE BATTERY CHEMISTRIES
25	Dong Yun Shin FLEXIBLE HOFMANN-TYPE METAL-ORGANIC FRAMEWORKS FOR XE STORAGE: A MOLECULAR DYNAMICS APPROACH BASED ON MACHINE LEARNING POTENTIAL
26	Electra Manoura THEORETICAL INVESTIGATION OF MOF'S LINKER FUNCTIONALIZATION FOR ENHANCING DESALINATION
27	Emmanuel Klontzas SIMULATION STUDIES OF VOLATILE ORGANIC COMPOUNDS ADSORPTION AND SEPARATION BY METAL- ORGANIC FRAMEWORK MIL-101(CR).
28	Feride Neva Yungul INTEGRATING MOLECULAR SIMULATIONS AND MACHINE LEARNING TO ASSESS MEMBRANE-BASED ${\rm CO_2/N_2}$ AND ${\rm O_2/N_2}$ SEPARATION PERFORMANCES OF METAL-ORGANIC FRAMEWORKS
29	Filip Sebesta REFINEMENT OF B18H22 CLUSTER AND CYCLOHEXANE ARRANGEMENT IN MOF PORES USING THE HYBRID QM/MM APPROACH
30	Florian Unterkofler APPLYING MACHINE-LEARNING APPROACHES FOR A QUANTITATIVELY RELIABLE DESCRIPTION OF HEAT TRANSPORT IN MOFS
31	Georgiy Baroncha RELATING PHASE TRANSITIONS OF CONFINED MATERIALS AND TOPOLOGY OF PORE NETWORK
32	Hyo-Sun Jang EFFECT OF OPEN METAL SITES ON METHANE ADSORPTION IN HKUST-1

33	Joy Ekka TOLUENE DETECTION AND CAPTURE USING MOF/POLYMER COMPOSITES
34	Kim Kirschenberger SEMI-REACTIVE FORCE FIELD FOR ZEOLITIC IMIDAZOLATE FRAMEWORKS
35	Li Wei Hsiao ANALYZING MOLECULE TRANSPORT IN MOF MATERIALS USING KINETIC MONTE CARLO SIMULATION
36	Mario Antonio Ongkiko SIMULATING 23NA NMR OF SODIUM-ION-MODIFIED ZIF-62 GLASS
37	Maryam Mansoori Kermani FUNCTIONALIZING THE STRUCTURE OF COFS TO ENHANCE THEIR CO ₂ UPTAKE CAPABILITY
38	Mattia Raimondo FROM HYBRID DFT FUNCTIONALS TO MACHINE LEARNING INTERATOMIC POTENTIALS FOR MOF
39	Minggao Feng A UNIVERSAL FOUNDATION MODEL FOR TRANSFER LEARNING IN MOLECULAR CRYSTALS
40	Mingyu Jeon METHANOL-ETHANOL DISCRIMINATION AND SELECTIVE SENSING ENABLED BY MOLECULAR SIEVING IN A CONDUCTIVE MOFS
41	Miroslav Pospíšil STUDY OF BORON CLUSTERS AND CYCLOHEXANE MOLECULES ANCHORING IN MOF BY MOLECULAR DYNAMICS
42	Nils Clovin ESTABLISHING MATERIAL-TRANSFERABLE DESIGN RULES FOR DEFECTIVE METAL-ORGANIC FRAMEWORKS AND METAL HALIDE PEROVSKITES THROUGH STRAIN ENGINEERING
43	Nils Holz TOWARDS A BENCHMARK FOR MACHINE LEARNING IN MOF SYNTHESIS: INTELLIGENT EXPLORATION OF PARAMETER SPACE
44	Nour Alkhatib UNDERSTANDING STRUCTURAL CHARACTERISTICS OF WATER IN CONFINEMENT
45	Pieter Dobbelaere CLUSTER-BASED LEARNING TO DESCRIBE DISORDERED METAL-ORGANIC FRAMEWORKS AT THE MESOSCALE
46	Prantar Dutta METAL-ORGANIC FRAMEWORKS FOR HYDROGEN/METHANE SEPARATION
47	Prathami Divakar Kamath MACHINE LEARNED POTENTIAL FOR HIGH-THROUGHPUT PHONON CALCULATIONS OF METAL-ORGANIC FRAMEWORKS
48	Thomas Nicholas MODELLING ELUSIVE ORDER-DISORDER PHASE TRANSITIONS IN METAL-ORGANIC FRAMEWORKS
49	Yizhi Xu PROBING THE ROLES OF SOLVENTS INSIDE METAL-ORGANIC FRAMEWORKS VIA MOLECULAR DYNAMICS SIMULATIONS

50	Alechania Misturini SOLVENT-RESPONSIVE PYRAZOLATE PEPTIDE FRAMEWORKS: NAVIGATING THEIR THERMODYNAMIC LANDSCAPE
51	$ \begin{array}{l} \textbf{Timur Biktagirov} \\ \textbf{FIRST-PRINCIPLES MODELING AND ESR IDENTIFICATION OF A NATIVE LINKER-BASED RADICAL IN UIO-66-NH_2 WITH QUANTUM SENSING FUNCTIONALITY \\ \end{array} $
52	Andrea Le Donne NANOCONFINED WATER IN HYBRID ZIF-7-8 MOF: A MOLECULAR-LEVEL PERSPECTIVE
53	Aparajita Ghosh COMPUTATIONAL SCREENING OF ZEOLITIC IMIDAZOLATE FRAMEWORKS (ZIFS) FOR OPTICAL SENSING OF VOCS VIA REFRACTIVE INDEX MODULATION
54	Beatriz Mouriño IMPACT OF ELECTRON-PHONON COUPLING AND EXCITONIC EFFECTS ON A BI-MOF PHOTOCATALYST FROM FIRST PRINCIPLES
55	Hilal Özyurt HIGH-THROUGHPUT ASSESSMENT OF GAS ADSORPTION IN THE REDD-COFFEES DATABASE USING MONTE CARLO SIMULATIONS AND MACHINE LEARNING
56	Erik Rohloff MODELLING OF ADSORPTION IN METAL-ORGANIC-FRAMEWORKS USING ATOMISTIC FORCE FIELDS
57	Felipe Lopes de Oliveira DECODING THE SYNERGISTIC ROLES OF AMINES AND PORE CONFINEMENT IN ${\rm CO_2}$ CHEMISORPTION BY COFS
58	Sabrina Grigoletto HIGH-PERFORMANCE HYDROPHOBIC MOFS FOR SELECTIVE ACETONE CAPTURE UNDER HUMID CONDITIONS
59	Samuel Greene SIMULATING WATER ADSORPTION IN METAL-ORGANIC FRAMEWORKS USING MONTE CARLO AND MACHINE LEARNING INTERATOMIC POTENTIALS
60	Satyanarayana Bonakala BRIDGING GENERIC FORCE FIELDS AND UNIVERSAL MACHINE LEARNING POTENTIALS FOR MOF SCREENING: ETHYLENE CAPTURE IN FOOD APPLICATIONS AS A BENCHMARK
61	Hooman Hasheminejad THE NEGLECTED ROLE OF THE SURFACE EXPOSURE OF MOFS IN SIMULATING WATER ADSORPTION FOR ATMOSPHERIC WATER HARVESTING
62	Valerii Karpov DFT ANALYSIS OF WATER DIFFUSION IN MOF-303
63	Mohammad Wahiduzzaman TUNING WATER ADSORPTION PROPERTIES OF MOFS
64	Sofia Kolin IMPACT OF PROLINE-FUNCTIONALIZED LINKERS ON DIFFUSION IN UIO-67 FRAMEWORKS - INSIGHTS FROM MOLECULAR DYNAMICS SIMULATIONS
65	Martin Attfield NANOSCALE FLEXING MECHANISM OF METAL-ORGANIC FRAMEWORK GA-MIL 53 REVEALED BY IN-SITU ATOMIC FORCE MICROSCOPY
66	Ahmed Gamai Attallah EXPLORING CO ₂ CAPTURE DYNAMICS IN CALF-20 MOFS USING POSITRON ANNIHILATION LIFETIME SPECTROSCOPY

67	Guangyuan Feng ELECTRIC-FIELD-MEDIATED IN-PLANE HETEROJUNCTION OF 2D COVALENT ORGANIC FRAMEWORKS
68	Maciej Grzywa ADVANCED DIFFRACTION TECHNIQUES FOR MOF STRUCTURAL ANALYSIS
69	Marta Przybyl LIQUID-PHASE IN SITU CRYSTALLIZATION AND CHARACTERIZATION USING ELECTRON MICROSCOPY AND DIFFRACTION
70	Mehrdad Asgari DEFECT INDUCED ANISOTROPIC NODE DISTORTION IN AMORPHOUS MOFS: LOW-VALENT ZR SITES AS CATALYTIC HOTSPOTS
71	Rebecca E. Reber REAL-TIME INVESTIGATION OF METAL-ORGANIC-FRAMEWORK SYNTHESIS VIA ULTRASOUND ATTENUATION AND SPECTROSCOPY
72	Ruirui Zhang TOWARD A COMPREHENSIVE IN-SITU UNDERSTANDING OF PD/HKUST-1-DERIVED PD/CUO CATALYSTS FOR CO OXIDATION
73	Russell Main USING ELECTRON DIFFRACTION TO UNLOCK THE CRYSTALLINE SPONGE TECHNIQUE
74	Thokozile Kathyola PRESSURE-INDUCED STRUCTURAL TRANSITIONS IN ZEOLITIC IMIDAZOLATE FRAMEWORKS
75	Valeryia Kasneryk INSIDE THE PROCESS OF FORMATION OF ZIF-8@ZN-AL LDH CONVERSION COATINGS ON SURFACE OF AA2024 ALLOY
76	Vera Butova FTIR STUDY OF SULFATED ZIRCONIA AND UIO-66: COORDINATION MODES AND ACTIVE SITE ACCESSIBILITY
77	Loïc Rochez-Ladeuze ADSORPTION OF NITROUS OXIDE IN ULTRAMICROPOROUS MAGNESIUM GALLATE
78	Zohrab Ahmadi DEMONSTRATING ZERO SECONDARY EMISSIONS FROM CALF-20 IN SVANTE'S VELOXOTHERM™ CO₂ CAPTURE PROCESS
79	Jikson Pulparayil Mathew A PRACTICAL AND ROBUST APPROACH TO DETERMINING THE EXPERIMENTAL MINIMAL FORMULA OF METAL-ORGANIC FRAMEWORKS.
80	Marco Ballabio HIGH CARRIER MOBILITY IN TRIPHENYLENEHEXATHIOL BASED METAL ORGANIC FRAMEWORKS MEASURED WITH TIME-RESOLVED TERAHERTZ SPECTROSCOPY
81	Nina Strasser THE ROLE OF CHEMICAL BONDING AND HYDRATION STATE ON THERMAL EXPANSION OF A ZINC-BASED METAL-ORGANIC FRAMEWORK
82	Giulia Taini ATOMIC-LEVEL INSIGHTS INTO CO_2 ADSORPTION IN A DEFECTIVE AMINO-FUNCTIONALIZED MOF THROUGH IN SITU HR-PXRD

83	Rafael Cortez Sgroi Pupo C-H ACTIVATION WITH CU(I) MOFs: THE PERTIMENCE OF NATURAL-LIKE ACTIVE CENTERS AND THEIR FACILE MODIFICATION
84	Jianbo Song FINE STRUCTURE OF A REDOX ACTIVE METAL-ORGANIC FRAMEWORK UPON 3D ELECTRON DIFFRACTION
85	Diletta Morelli Venturi STABILITY AND REDOX BEHAVIOR OF CERIUM-BASED MOFS UNDER NON-THERMAL PLASMA CONDITIONS FOR CO_2 HYDROGENATION
86	Fabio André Peixoto Esteves DIAMINE-APPENDED METAL-ORGANIC FRAMEWORKS PROMOTE THE HYDROGENATION OF CO₂ TO METHANOL AT LOW PARTIAL PRESSURES
87	Marika Di Berto Mancini ILLUMINATING CHARGE TRANSFER MECHANISMS IN PHOTOACTIVE MOFS DURING CO ₂ PHOTOREDUCTION
88	Nina Lock CORRELATING THE STRUCTURAL TRANSFORMATION AND ELECTROCATALYTIC PROPERTIES OF ZIF-67 DURING PYROLYSIS
89	Anna Liutkova UIO-66 SUPPORTED COPPER-ZINC CATALYSTS FOR CARBON DIOXIDE-TO-METHANOL CONVERSION: STRUCTURE-ACTIVITY INSIGHTS FROM IN SITU X-RAY STUDIES
90	Mathilde Lepoitevin METAL-ORGANIC FRAMEWORKS FOR ENHANCED ANTIBACTERIAL WOUND HEALING
91	Isabel del Castillo-Velilla DECIPHERING INTERFACIAL INTERACTIONS IN A DUAL-FUNCTIONAL MOF@COF COMPOSITE FOR WATER REMEDIATION
92	Pooja Sindhu MOF-ON-MOF HETEROSTRUCTURE THIN FILM: A RATIONAL DESIGN STRATEGY TO INVESTIGATE EMERGENT INTERFACIAL PHENOMENA
93	Annette Vollrath IN SITU ENTRAPMENT OF MR-TADF EMITTER DIKTA IN METAL-ORGANIC FRAMEWORK MOF-5 AND THEIR PHOTOPHYSICAL PROPERTIES
94	Joohan Nam STRUCTURE-INFORMED MODULATION OF ZEOLITIC IMIDAZOLATE FRAMEWORKS
95	Kunyi Leng CONTROLLING THE SELF-ASSEMBLY AND MECHANICAL PROPERTIES OF ISOSTRUCTURAL DISULFIDE- BASED METAL-ORGANIC NANOTUBES
96	Liyuan Qu MODULATING INTRINSIC CHARGE MOBILITY VIA MANIPULATING Π-Π INTERACTION DISTANCES IN THREE ISOSTRUCTURAL POROUS MOLECULAR CONDUCTORS
97	Shuo Sun COVALENT ORGANIC FRAMEWORK EMBEDDED WITH SINGLE CU-SITES FOR PHOTOCATALYTIC REACTION
98	Zhenyu Zhao LUMINESCENT LANTHANIDE-BASED METAL-ORGANIC FRAMEWORKS AS AMBIENT OXYGEN GAS SENSORS WITH RAPID RESPONSE

99	Mariana Bessa DUAL-PSA PROCESS FOR THE SEPARATION OF H_2 , CH_4 , AND C_2H_6 WITH THE MOF MIL-100(FE)
100	Antonia Mosberger DEVELOPMENT OF A NOVEL MG-FUMARATE MOF (DUT-153) WITH EXTRAORDINARY TUNABILITY OF ADSORPTION PROPERTIES
101	Bhawna Kumari CRYSTAL ENGINEERING SQUARE-LATTICE COORDINATION NETWORKS FOR ATMOSPHERIC WATER HARVESTING
102	Chaewon Shin DEFECT-ENGINEERED HKUST-1 WITH CU(I) SITES FOR ENHANCED HYDROGEN STORAGE
103	David Farrusseng HOW TO ASSESS THE THERMODYNAMIC EQUILIBRIUM OF ADSORPTION FOR IN-VACUUM DECONTAMINATION
104	Nuttaporn Krittametaporn LUMINESCENT MOF GLASSES VIA LIQUID PHASE MIXING WITH CHELATING ORGANIC LUMINOPHORE COLIGANDS
105	Ioannis Bratsos AN HETEROMETALLIC CU(II)-PD(II) MOF FOR CO₂ CAPTURE AND CH₄ STORAGE
106	Herald Paja MACHINE LEARNING DERIVED ATOMIC CHARGES OF METAL- ORGANIC FRAMEWORKS FROM A WELL-CURATED SMALL DATASET
107	Vladimir Shirobokov MACHINE LEARNING APPROACH FOR PREDICTION SECOND HARMONIC GENERATION IN METAL-ORGANIC FRAMEWORKS