	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 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 CO_2/N_2 AND 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	**Timur Biktagirov** FIRST-PRINCIPLES MODELING AND ESR IDENTIFICATION OF A NATIVE LINKER-BASED RADICAL IN UIO-66-NH_2 WITH QUANTUM SENSING FUNCTIONALITY
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 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 Gamal 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™ CO_2 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	**Petra Agota Szilagyi** PERFORMANCE AND NANOCONFINEMENT EFFECTS IN PD/UIO CATALYSTS FOR THE DIRECT CO_2-TO-METHANOL HYDROGENATION
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 CO_2 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 CO_2 CAPTURE AND CH_4 STORAGE