Jihan Kim

List of Publications by Year in Descending Order

79 papers	3,804 citations	26 h-index	61 g-index
85 ext. papers	4,828 ext. citations	10.3 avg, IF	5.78 L-index

#	Paper	IF	Citations
79	Oxide/ZIF-8 Hybrid Nanofiber Yarns: Heightened Surface Activity for Exceptional Chemiresistive Sensing.. *Advanced Materials*, **2022**, e2105869	24	2
78	Mining Insights on Metal-Organic Framework Synthesis from Scientific Literature Texts.. *Journal of Chemical Information and Modeling*, **2022**, 62, 1190-1198	6.1	0
77	Tunable Electrical Conductivity of Flexible Metal□Organic Frameworks. *Chemistry of Materials*, **2022**, 34, 254-265	9.6	1
76	Computational Identification of Connected MOF@COF Materials. *Journal of Physical Chemistry C*, **2021**, 125, 5897-5903	3.8	4
75	Exploring Guest-Dependent Photoconductivity in a Donor-Containing Metal□Organic Framework. *Journal of Physical Chemistry C*, **2021**, 125, 10198-10206	3.8	2
74	Polyelemental Nanoparticles as Catalysts for a Li-O Battery. *ACS Nano*, **2021**, 15, 4235-4244	16.7	18
73	Computational Screening of Trillions of Metal-Organic Frameworks for High-Performance Methane Storage. *ACS Applied Materials & Interfaces*, **2021**, 13, 23647-23654	9.5	20
72	Innentitelbild: Void Space versus Surface Functionalization for Proton Conduction in Metal□Organic Frameworks (Angew. Chem. 37/2021). *Angewandte Chemie*, **2021**, 133, 20226-20226	3.6	
71	Void Space versus Surface Functionalization for Proton Conduction in Metal-Organic Frameworks. *Angewandte Chemie - International Edition*, **2021**, 60, 20173-20177	16.4	7
70	New model for S-shaped isotherm data and its application to process modeling using IAST. *Chemical Engineering Journal*, **2021**, 420, 127580	14.7	1
69	Finely tuned inverse design of metal□rganic frameworks with user-desired Xe/Kr selectivity. *Journal of Materials Chemistry A*, **2021**, 9, 21175-21183	13	1
68	Gas Adsorption Enhancement in Partially Amorphized Metal□Organic Frameworks. *Journal of Physical Chemistry C*, **2021**, 125, 4509-4518	3.8	3
67	Deep learning-based initial guess for minimum energy path calculations. *Korean Journal of Chemical Engineering*, **2021**, 38, 406-410	2.8	0
66	Void Space versus Surface Functionalization for Proton Conduction in Metal□Organic Frameworks. *Angewandte Chemie*, **2021**, 133, 20335-20339	3.6	0
65	Confinement of Ultrasmall Bimetallic Nanoparticles in Conductive Metal-Organic Frameworks via Site-Specific Nucleation. *Advanced Materials*, **2021**, 33, e2101216	24	6
64	Confinement of Ultrasmall Bimetallic Nanoparticles in Conductive Metal□Organic Frameworks via Site-Specific Nucleation (Adv. Mater. 38/2021). *Advanced Materials*, **2021**, 33, 2170302	24	0
63	Machine learning-based discovery of molecules, crystals, and composites: A perspective review. *Korean Journal of Chemical Engineering*, **2021**, 38, 1971-1982	2.8	1

62	Computational Design of a Photoresponsive Metal Organic Framework for Post Combustion Carbon Capture. *Journal of Physical Chemistry C*, **2020**, 124, 13162-13167	3.8	10
61	Understanding Reaction Pathways in High Dielectric Electrolytes Using MoC as a Catalyst for Li-CO Batteries. *ACS Applied Materials & Interfaces*, **2020**, 12, 32633-32641	9.5	7
60	Highly durable metal ensemble catalysts with full dispersion for automotive applications beyond single-atom catalysts. *Nature Catalysis*, **2020**, 3, 368-375	36.5	87
59	Finding Hidden Signals in Chemical Sensors Using Deep Learning. *Analytical Chemistry*, **2020**, 92, 6529-6537	7.8	18
58	Self-operating transpiration-driven electrokinetic power generator with an artificial hydrological cycle. *Energy and Environmental Science*, **2020**, 13, 527-534	35.4	45
57	Rational modifications of PCN-700 to induce electrical conductivity: a computational study. *Dalton Transactions*, **2020**, 49, 102-113	4.3	6
56	Inverse design of porous materials using artificial neural networks. *Science Advances*, **2020**, 6, eaax9324	14.3	79
55	Isotherm parameter library and evaluation software for CO2 capture adsorbents. *Computers and Chemical Engineering*, **2020**, 143, 107105	4	6
54	Applications of machine learning in metal-organic frameworks. *Coordination Chemistry Reviews*, **2020**, 423, 213487	23.2	51
53	2D Materials Decorated with Ultrathin and Porous Graphene Oxide for High Stability and Selective Surface Activity. *Advanced Materials*, **2020**, 32, e2002723	24	18
52	Reverse shape selectivity of hexane isomer in ligand inserted MOF-74.. *RSC Advances*, **2020**, 10, 22601-22605	3.7	3
51	Ultrathin Magnesium Nanosheet for Improved Hydrogen Storage with Fishbone Shaped One-Dimensional Carbon Matrix. *ACS Applied Energy Materials*, **2020**, 3, 8143-8149	6.1	6
50	Photochemically Induced Water Harvesting in Metal Organic Framework. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 15854-15859	8.3	15
49	Predicting performance limits of methane gas storage in zeolites with an artificial neural network. *Journal of Materials Chemistry A*, **2019**, 7, 2709-2716	13	19
48	Ultra-dense (~20 Tdot/in) nanoparticle array from an ordered supramolecular dendrimer containing a metal precursor. *Scientific Reports*, **2019**, 9, 3885	4.9	1
47	Computational Analysis of Linker Defective Metal-Organic Frameworks for Membrane Separation Applications. *Langmuir*, **2019**, 35, 3917-3924	4	5
46	Computer-aided discovery of connected metal-organic frameworks. *Nature Communications*, **2019**, 10, 3620	17.4	38
45	Formation of toroidal LiO in non-aqueous Li-O batteries with MoCT MXene/CNT composite.. *RSC Advances*, **2019**, 9, 41120-41125	3.7	8

44	Polyelemental Nanolithography via Plasma Ion Bombardment: From Fabrication to Superior H Sensing Application. *Advanced Materials*, **2019**, 31, e1805343	24	22
43	Transferability of CO2 Force Fields for Prediction of Adsorption Properties in All-Silica Zeolites. *Journal of Physical Chemistry C*, **2018**, 122, 10892-10903	3.8	11
42	Metallic TiCT MXene Gas Sensors with Ultrahigh Signal-to-Noise Ratio. *ACS Nano*, **2018**, 12, 986-993	16.7	664
41	Energy-efficient CO hydrogenation with fast response using photoexcitation of CO adsorbed on metal catalysts. *Nature Communications*, **2018**, 9, 3027	17.4	54
40	Shift of the Branching Point of the Side-Chain in Naphthalenediimide (NDI)-Based Polymer for Enhanced Electron Mobility and All-Polymer Solar Cell Performance. *Advanced Functional Materials*, **2018**, 28, 1803613	15.6	58
39	Rational Design of Aminopolymer for Selective Discrimination of Acidic Air Pollutants. *ACS Sensors*, **2018**, 3, 1329-1337	9.2	9
38	Text Mining Metal-Organic Framework Papers. *Journal of Chemical Information and Modeling*, **2018**, 58, 244-251	6.1	26
37	User-friendly graphical user interface software for ideal adsorbed solution theory calculations. *Korean Journal of Chemical Engineering*, **2018**, 35, 214-221	2.8	50
36	Molybdenum carbide chemical sensors with ultrahigh signal-to-noise ratios and ambient stability. *Journal of Materials Chemistry A*, **2018**, 6, 23408-23416	13	21
35	Edge-Functionalized Graphene Nanoribbon Chemical Sensor: Comparison with Carbon Nanotube and Graphene. *ACS Applied Materials & Interfaces*, **2018**, 10, 42905-42914	9.5	28
34	Ligand Insertion in MOF-74 as Effective Design for Oxidation of Ethane to Ethanol. *Journal of Physical Chemistry C*, **2018**, 122, 23078-23083	3.8	14
33	Influence of graphene thickness and grain boundaries on MoS wrinkle nanostructures. *Physical Chemistry Chemical Physics*, **2018**, 20, 17000-17008	3.6	7
32	Surface Plasmon Aided Ethanol Dehydrogenation Using AgNi Binary Nanoparticles. *ACS Catalysis*, **2017**, 7, 2294-2302	13.1	32
31	Materials Genome in Action: Identifying the Performance Limits of Physical Hydrogen Storage. *Chemistry of Materials*, **2017**, 29, 2844-2854	9.6	123
30	Understanding gas adsorption in MOF-5/graphene oxide composite materials. *Physical Chemistry Chemical Physics*, **2017**, 19, 11639-11644	3.6	18
29	Computational prediction of hetero-interpenetration in metal-organic frameworks. *Chemical Communications*, **2017**, 53, 1953-1956	5.8	12
28	Size-Matching Ligand Insertion in MOF-74 for Enhanced CO2 Capture under Humid Conditions. *Journal of Physical Chemistry C*, **2017**, 121, 24444-24451	3.8	24
27	Computational prediction of high methane storage capacity in V-MOF-74. *Physical Chemistry Chemical Physics*, **2017**, 19, 21132-21139	3.6	12

26	Excavating hidden adsorption sites in metal-organic frameworks using rational defect engineering. *Nature Communications*, **2017**, 8, 1539	17.4	36
25	Modeling adsorption properties of structurally deformed metal-organic frameworks using structure-property map. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 7923-7928	11.5	19
24	High-throughput computational screening of nanoporous adsorbents for CO2 capture from natural gas. *Molecular Systems Design and Engineering*, **2016**, 1, 175-188	4.6	37
23	Towards accurate porosity descriptors based on guest-host interactions. *Journal of Molecular Graphics and Modelling*, **2016**, 66, 91-8	2.8	1
22	Tuning the electrode work function via a vapor-phase deposited ultrathin polymer film. *Journal of Materials Chemistry C*, **2016**, 4, 831-839	7.1	9
21	Superior Chemical Sensing Performance of Black Phosphorus: Comparison with MoS2 and Graphene. *Advanced Materials*, **2016**, 28, 7020-8	24	267
20	Thermodynamics of gas adsorption in MOFs using Ab Initio calculations. *International Journal of Quantum Chemistry*, **2016**, 116, 569-572	2.1	8
19	Understanding the Mechanisms of CO2 Adsorption Enhancement in Pure Silica Zeolites under Humid Conditions. *Journal of Physical Chemistry C*, **2016**, 120, 23500-23510	3.8	27
18	Probing gas adsorption in MOFs using an efficient ab initio widom insertion Monte Carlo method. *Journal of Computational Chemistry*, **2016**, 37, 2808-2815	3.5	6
17	Highly Enhanced Gas Adsorption Properties in Vertically Aligned MoS2 Layers. *ACS Nano*, **2015**, 9, 9314-21	16.7	310
16	The materials genome in action: identifying the performance limits for methane storage. *Energy and Environmental Science*, **2015**, 8, 1190-1199	35.4	263
15	Computational structure characterization tools for the era of material informatics. *Chemical Engineering Science*, **2015**, 121, 322-330	4.4	21
14	Predicting low-k zeolite materials. *Journal of Materials Chemistry C*, **2014**, 2, 2298-2300	7.1	8
13	Optimizing nanoporous materials for gas storage. *Physical Chemistry Chemical Physics*, **2014**, 16, 5499-513	3.6	67
12	Efficient Determination of Accurate Force Fields for Porous Materials Using ab Initio Total Energy Calculations. *Journal of Physical Chemistry C*, **2014**, 118, 2693-2701	3.8	21
11	Computational generation of user-desired multivariate metal-organic framework structures. *ChemPhysChem*, **2014**, 15, 61-3	3.2	1
10	Evaluating mixture adsorption models using molecular simulation. *AICHE Journal*, **2013**, 59, 3054-3064	3.6	23
9	New materials for methane capture from dilute and medium-concentration sources. *Nature Communications*, **2013**, 4, 1694	17.4	84

8	Predicting large CO2 adsorption in aluminosilicate zeolites for postcombustion carbon dioxide capture. *Journal of the American Chemical Society*, **2012**, 134, 18940-3	16.4	114
7	High-Throughput Characterization of Porous Materials Using Graphics Processing Units. *Journal of Chemical Theory and Computation*, **2012**, 8, 1684-93	6.4	53
6	Ab initio carbon capture in open-site metal-organic frameworks. *Nature Chemistry*, **2012**, 4, 810-6	17.6	263
5	In silico screening of carbon-capture materials. *Nature Materials*, **2012**, 11, 633-41	27	433
4	Efficient Monte Carlo Simulations of Gas Molecules Inside Porous Materials. *Journal of Chemical Theory and Computation*, **2012**, 8, 2336-43	6.4	31
3	Molecular Monte Carlo Simulations Using Graphics Processing Units: To Waste Recycle or Not?. *Journal of Chemical Theory and Computation*, **2011**, 7, 3208-22	6.4	22
2	Computational techniques for characterisation of electrically conductive MOFs: quantum calculations and machine learning approaches. *Journal of Materials Chemistry C*,	7.1	0
1	Suppressing Charge Disproportionation of MnO2 Cathodes in Rechargeable Zinc Ion Batteries via Cooperative Jahn-Teller Distortion. *Batteries and Supercaps*,	5.6	1