## Jihan Kim

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Metallic Ti <sub>3</sub> C <sub>2</sub> T <sub><i>x</i></sub> MXene Gas Sensors with Ultrahigh Signal-to-Noise Ratio. ACS Nano, 2018, 12, 986-993.	7.3	1,153
2	In silico screening of carbon-capture materials. Nature Materials, 2012, 11, 633-641.	13.3	497
3	Highly Enhanced Gas Adsorption Properties in Vertically Aligned MoS <sub>2</sub> Layers. ACS Nano, 2015, 9, 9314-9321.	7.3	417
4	Superior Chemical Sensing Performance of Black Phosphorus: Comparison with MoS <sub>2</sub> and Graphene. Advanced Materials, 2016, 28, 7020-7028.	11.1	355
5	The materials genome in action: identifying the performance limits for methane storage. Energy and Environmental Science, 2015, 8, 1190-1199.	15.6	314
6	Ab initio carbon capture in open-site metal–organic frameworks. Nature Chemistry, 2012, 4, 810-816.	6.6	310
7	Highly durable metal ensemble catalysts with full dispersion for automotive applications beyond single-atom catalysts. Nature Catalysis, 2020, 3, 368-375.	16.1	220
8	Inverse design of porous materials using artificial neural networks. Science Advances, 2020, 6, eaax9324.	4.7	171
9	Materials Genome in Action: Identifying the Performance Limits of Physical Hydrogen Storage. Chemistry of Materials, 2017, 29, 2844-2854.	3.2	169
10	Predicting Large CO <sub>2</sub> Adsorption in Aluminosilicate Zeolites for Postcombustion Carbon Dioxide Capture. Journal of the American Chemical Society, 2012, 134, 18940-18943.	6.6	129
11	Self-operating transpiration-driven electrokinetic power generator with an artificial hydrological cycle. Energy and Environmental Science, 2020, 13, 527-534.	15.6	122
12	New materials for methane capture from dilute and medium-concentration sources. Nature Communications, 2013, 4, 1694.	5.8	111
13	Applications of machine learning in metal-organic frameworks. Coordination Chemistry Reviews, 2020, 423, 213487.	9.5	100
14	User-friendly graphical user interface software for ideal adsorbed solution theory calculations. Korean Journal of Chemical Engineering, 2018, 35, 214-221.	1.2	88
15	Energy-efficient CO2 hydrogenation with fast response using photoexcitation of CO2 adsorbed on metal catalysts. Nature Communications, 2018, 9, 3027.	5.8	86
16	Computational Screening of Trillions of Metal–Organic Frameworks for High-Performance Methane Storage. ACS Applied Materials & Interfaces, 2021, 13, 23647-23654.	4.0	81
17	Optimizing nanoporous materials for gas storage. Physical Chemistry Chemical Physics, 2014, 16, 5499.	1.3	76
18	Shift of the Branching Point of the Sideâ€Chain in Naphthalenediimide (NDI)â€Based Polymer for Enhanced Electron Mobility and Allâ€Polymer Solar Cell Performance. Advanced Functional Materials, 2018, 28, 1803613.	7.8	74

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19	Computer-aided discovery of connected metal-organic frameworks. Nature Communications, 2019, 10, 3620.	5.8	71
20	Excavating hidden adsorption sites in metal-organic frameworks using rational defect engineering. Nature Communications, 2017, 8, 1539.	5.8	60
21	High-Throughput Characterization of Porous Materials Using Graphics Processing Units. Journal of Chemical Theory and Computation, 2012, 8, 1684-1693.	2.3	57
22	High-throughput computational screening of nanoporous adsorbents for CO <sub>2</sub> capture from natural gas. Molecular Systems Design and Engineering, 2016, 1, 175-188.	1.7	54
23	Text Mining Metal–Organic Framework Papers. Journal of Chemical Information and Modeling, 2018, 58, 244-251.	2.5	43
24	Surface Plasmon Aided Ethanol Dehydrogenation Using Ag–Ni Binary Nanoparticles. ACS Catalysis, 2017, 7, 2294-2302.	5.5	42
25	Edge-Functionalized Graphene Nanoribbon Chemical Sensor: Comparison with Carbon Nanotube and Graphene. ACS Applied Materials & Interfaces, 2018, 10, 42905-42914.	4.0	41
26	Finding Hidden Signals in Chemical Sensors Using Deep Learning. Analytical Chemistry, 2020, 92, 6529-6537.	3.2	40
27	Polyelemental Nanolithography via Plasma Ion Bombardment: From Fabrication to Superior H <sub>2</sub> Sensing Application. Advanced Materials, 2019, 31, e1805343.	11.1	38
28	Polyelemental Nanoparticles as Catalysts for a Li–O <sub>2</sub> Battery. ACS Nano, 2021, 15, 4235-4244.	7.3	38
29	Efficient Monte Carlo Simulations of Gas Molecules Inside Porous Materials. Journal of Chemical Theory and Computation, 2012, 8, 2336-2343.	2.3	36
30	Molybdenum carbide chemical sensors with ultrahigh signal-to-noise ratios and ambient stability. Journal of Materials Chemistry A, 2018, 6, 23408-23416.	5.2	35
31	Size-Matching Ligand Insertion in MOF-74 for Enhanced CO <sub>2</sub> Capture under Humid Conditions. Journal of Physical Chemistry C, 2017, 121, 24444-24451.	1.5	34
32	Understanding the Mechanisms of CO <sub>2</sub> Adsorption Enhancement in Pure Silica Zeolites under Humid Conditions. Journal of Physical Chemistry C, 2016, 120, 23500-23510.	1.5	33
33	Predicting performance limits of methane gas storage in zeolites with an artificial neural network. Journal of Materials Chemistry A, 2019, 7, 2709-2716.	5.2	33
34	2D Materials Decorated with Ultrathin and Porous Graphene Oxide for High Stability and Selective Surface Activity. Advanced Materials, 2020, 32, e2002723.	11.1	33
35	Void Space versus Surface Functionalization for Proton Conduction in Metal–Organic Frameworks. Angewandte Chemie - International Edition, 2021, 60, 20173-20177.	7.2	32
36	Evaluating mixture adsorption models using molecular simulation. AICHE Journal, 2013, 59, 3054-3064.	1.8	31

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37	Computational structure characterization tools for the era of material informatics. Chemical Engineering Science, 2015, 121, 322-330.	1.9	29
38	Oxide/ZIFâ€8 Hybrid Nanofiber Yarns: Heightened Surface Activity for Exceptional Chemiresistive Sensing. Advanced Materials, 2022, 34, e2105869.	11.1	29
39	Mining Insights on Metal–Organic Framework Synthesis from Scientific Literature Texts. Journal of Chemical Information and Modeling, 2022, 62, 1190-1198.	2.5	27
40	Understanding gas adsorption in MOF-5/graphene oxide composite materials. Physical Chemistry Chemical Physics, 2017, 19, 11639-11644.	1.3	24
41	Photochemically Induced Water Harvesting in Metal–Organic Framework. ACS Sustainable Chemistry and Engineering, 2019, 7, 15854-15859.	3.2	24
42	Molecular Monte Carlo Simulations Using Graphics Processing Units: To Waste Recycle or Not?. Journal of Chemical Theory and Computation, 2011, 7, 3208-3222.	2.3	23
43	Efficient Determination of Accurate Force Fields for Porous Materials Using ab Initio Total Energy Calculations. Journal of Physical Chemistry C, 2014, 118, 2693-2701.	1.5	23
44	Confinement of Ultrasmall Bimetallic Nanoparticles in Conductive Metal–Organic Frameworks via Siteâ€6pecific Nucleation. Advanced Materials, 2021, 33, e2101216.	11.1	23
45	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.	3.3	22
46	Understanding Reaction Pathways in High Dielectric Electrolytes Using β-Mo <sub>2</sub> C as a Catalyst for Li–CO <sub>2</sub> Batteries. ACS Applied Materials & Interfaces, 2020, 12, 32633-32641.	4.0	22
47	N–p-Conductor Transition of Gas Sensing Behaviors in Mo <sub>2</sub> CT <sub><i>x</i></sub> MXene. ACS Sensors, 2022, 7, 2225-2234.	4.0	20
48	Ligand Insertion in MOF-74 as Effective Design for Oxidation of Ethane to Ethanol. Journal of Physical Chemistry C, 2018, 122, 23078-23083.	1.5	19
49	Finely tuned inverse design of metal–organic frameworks with user-desired Xe/Kr selectivity. Journal of Materials Chemistry A, 2021, 9, 21175-21183.	5.2	19
50	Computational prediction of hetero-interpenetration in metal–organic frameworks. Chemical Communications, 2017, 53, 1953-1956.	2.2	18
51	Computational Design of a Photoresponsive Metal–Organic Framework for Post Combustion Carbon Capture. Journal of Physical Chemistry C, 2020, 124, 13162-13167.	1.5	18
52	Suppressing Charge Disproportionation of MnO <sub>2</sub> Cathodes in Rechargeable Zinc Ion Batteries via Cooperative Jahnâ€Teller Distortion. Batteries and Supercaps, 2021, 4, 1881-1888.	2.4	17
53	Formation of toroidal Li <sub>2</sub> O <sub>2</sub> in non-aqueous Li–O <sub>2</sub> batteries with Mo <sub>2</sub> CT <sub>x</sub> MXene/CNT composite. RSC Advances, 2019, 9, 41120-41125.	1.7	16
54	Ultrathin Magnesium Nanosheet for Improved Hydrogen Storage with Fishbone Shaped One-Dimensional Carbon Matrix. ACS Applied Energy Materials, 2020, 3, 8143-8149.	2.5	16

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55	Computational prediction of high methane storage capacity in V-MOF-74. Physical Chemistry Chemical Physics, 2017, 19, 21132-21139.	1.3	14
56	Rational Design of Aminopolymer for Selective Discrimination of Acidic Air Pollutants. ACS Sensors, 2018, 3, 1329-1337.	4.0	14
57	Computational techniques for characterisation of electrically conductive MOFs: quantum calculations and machine learning approaches. Journal of Materials Chemistry C, 2021, 9, 13584-13599.	2.7	14
58	Interface-Sensitized Chemiresistor: Integrated Conductive and Porous Metal-Organic Frameworks. Chemical Engineering Journal, 2022, 449, 137780.	6.6	14
59	Transferability of CO <sub>2</sub> Force Fields for Prediction of Adsorption Properties in All-Silica Zeolites. Journal of Physical Chemistry C, 2018, 122, 10892-10903.	1.5	12
60	Computational Identification of Connected MOF@COF Materials. Journal of Physical Chemistry C, 2021, 125, 5897-5903.	1.5	12
61	Gas Adsorption Enhancement in Partially Amorphized Metal–Organic Frameworks. Journal of Physical Chemistry C, 2021, 125, 4509-4518.	1.5	11
62	Predicting low-k zeolite materials. Journal of Materials Chemistry C, 2014, 2, 2298-2300.	2.7	10
63	Thermodynamics of gas adsorption in <scp>MOF</scp> s using <i>Ab Initio</i> calculations. International Journal of Quantum Chemistry, 2016, 116, 569-572.	1.0	9
64	Tuning the electrode work function via a vapor-phase deposited ultrathin polymer film. Journal of Materials Chemistry C, 2016, 4, 831-839.	2.7	9
65	Influence of graphene thickness and grain boundaries on MoS <sub>2</sub> wrinkle nanostructures. Physical Chemistry Chemical Physics, 2018, 20, 17000-17008.	1.3	9
66	Isotherm parameter library and evaluation software for CO2 capture adsorbents. Computers and Chemical Engineering, 2020, 143, 107105.	2.0	9
67	New model for S-shaped isotherm data and its application to process modeling using IAST. Chemical Engineering Journal, 2021, 420, 127580.	6.6	9
68	Probing gas adsorption in MOFs using an efficient <i>ab initio</i> widom insertion Monte Carlo method. Journal of Computational Chemistry, 2016, 37, 2808-2815.	1.5	8
69	Computational Analysis of Linker Defective Metal–Organic Frameworks for Membrane Separation Applications. Langmuir, 2019, 35, 3917-3924.	1.6	8
70	Rational modifications of PCN-700 to induce electrical conductivity: a computational study. Dalton Transactions, 2020, 49, 102-113.	1.6	8
71	Reverse shape selectivity of hexane isomer in ligand inserted MOF-74. RSC Advances, 2020, 10, 22601-22605.	1.7	8
72	Rational Tuning of Ultramicropore Dimensions in MOF-74 for Size-Selective Separation of Light Hydrocarbons. Chemistry of Materials, 2021, 33, 7686-7692.	3.2	8

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73	Tunable Electrical Conductivity of Flexible Metal–Organic Frameworks. Chemistry of Materials, 2022, 34, 254-265.	3.2	7
74	Application of transfer learning to predict diffusion properties in metal–organic frameworks. Molecular Systems Design and Engineering, 2022, 7, 1056-1064.	1.7	7
75	Exploring Guest-Dependent Photoconductivity in a Donor-Containing Metal–Organic Framework. Journal of Physical Chemistry C, 2021, 125, 10198-10206.	1.5	6
76	Machine learning-based discovery of molecules, crystals, and composites: A perspective review. Korean Journal of Chemical Engineering, 2021, 38, 1971-1982.	1.2	4
77	Confinement of Ultrasmall Bimetallic Nanoparticles in Conductive Metal–Organic Frameworks via Site‣pecific Nucleation (Adv. Mater. 38/2021). Advanced Materials, 2021, 33, 2170302.	11.1	3
78	Void Space versus Surface Functionalization for Proton Conduction in Metal–Organic Frameworks. Angewandte Chemie, 2021, 133, 20335-20339.	1.6	2
79	Understanding the Structural Collapse during Activation of Metal–Organic Frameworks with Copper Paddlewheels. Inorganic Chemistry, 2022, 61, 9702-9709.	1.9	2
80	Computational Generation of Userâ€Desired Multivariate Metal–Organic Framework Structures. ChemPhysChem, 2014, 15, 61-63.	1.0	1
81	Towards accurate porosity descriptors based on guest-host interactions. Journal of Molecular Graphics and Modelling, 2016, 66, 91-98.	1.3	1
82	Ultra-dense (~20 Tdot/in2) nanoparticle array from an ordered supramolecular dendrimer containing a metal precursor. Scientific Reports, 2019, 9, 3885.	1.6	1
83	Deep learning-based initial guess for minimum energy path calculations. Korean Journal of Chemical Engineering, 2021, 38, 406-410.	1.2	1
84	Innentitelbild: Void Space versus Surface Functionalization for Proton Conduction in Metal–Organic Frameworks (Angew. Chem. 37/2021). Angewandte Chemie. 2021. 133. 20226-20226.	1.6	0