Tony Pham

List of Publications by Year in descending order

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112 papers	8,570 citations	66343 42 h-index	45317 90 g-index
114 all docs	114 docs citations	114 times ranked	5650 citing authors

#	Article	IF	Citations
1	Selfâ€Adjusting Metalâ€“Organic Framework for Efficient Capture of Trace Xenon and Krypton. Angewandte Chemie, 2022, 134, .	2.0	5
2	Selfâ€Adjusting Metalâ€“Organic Framework for Efficient Capture of Trace Xenon and Krypton. Angewandte Chemie - International Edition, 2022, 61, .	13.8	47
3	Investigating H₂ Adsorption in Isostructural Metalâ€“Organic Frameworks M-CUK-1 (M = Co) Tj ETQq1 1 0.784314 rgBT /C 14, 8126-8136.	8.0	5
4	Metalâ€“Organic Framework Based Hydrogen-Bonding Nanotrap for Efficient Acetylene Storage and Separation. Journal of the American Chemical Society, 2022, 144, 1681-1689.	13.7	172
5	Methane storage in flexible and dynamical metalâ€“organic frameworks. Chemical Physics Reviews, 2022, 3, .	5.7	7
6	Pore-Nanospace Engineering of Mixed-Ligand Metalâ€“Organic Frameworks for High Adsorption of Hydrofluorocarbons and Hydrochlorofluorocarbons. Chemistry of Materials, 2022, 34, 5116-5124.	6.7	11
7	A robust soc-MOF platform exhibiting high gravimetric uptake and volumetric deliverable capacity for on-board methane storage. Nano Research, 2021, 14, 512-517.	10.4	40
8	A robust heterometallic ultramicroporous MOF with ultrahigh selectivity for propyne/propylene separation. Journal of Materials Chemistry A, 2021, 9, 2850-2856.	10.3	22
9	A MOFâ€based Ultraâ€Strong Acetylene Nanoâ€trap for Highly Efficient C₂H₂/CO₂ Separation. Angewandte Chemie, 2021, 133, 5343-5348.	2.0	49
10	Frontispiz: A MOFâ€based Ultraâ€Strong Acetylene Nanoâ€trap for Highly Efficient C₂H₂/CO₂ Separation. Angewandte Chemie, 2021, 133, .	2.0	1
11	Frontispiece: A MOFâ€based Ultraâ€Strong Acetylene Nanoâ€trap for Highly Efficient C₂H₂/CO₂ Separation. Angewandte Chemie - International Edition, 2021, 60, .	13.8	0
12	A MOFâ€based Ultraâ€Strong Acetylene Nanoâ€trap for Highly Efficient C₂H₂/CO₂ Separation. Angewandte Chemie - International Edition, 2021, 60, 5283-5288.	13.8	172
13	Nanospace Engineering of Metalâ€“Organic Frameworks through Dynamic Spacer Installation of Multifunctionalities for Efficient Separation of Ethane from Ethane/Ethylene Mixtures. Angewandte Chemie, 2021, 133, 9766-9771.	2.0	9
14	Nanospace Engineering of Metalâ€“Organic Frameworks through Dynamic Spacer Installation of Multifunctionalities for Efficient Separation of Ethane from Ethane/Ethylene Mixtures. Angewandte Chemie - International Edition, 2021, 60, 9680-9685.	13.8	89
15	Aminoâ€Functionalised Hybrid Ultramicroporous Materials that Enable Singleâ€Step Ethylene Purification from a Ternary Mixture. Angewandte Chemie, 2021, 133, 10997-11004.	2.0	10
16	Aminoâ€Functionalised Hybrid Ultramicroporous Materials that Enable Singleâ€Step Ethylene Purification from a Ternary Mixture. Angewandte Chemie - International Edition, 2021, 60, 10902-10909.	13.8	56
17	Molecular Sieving of Acetylene from Ethylene in a Rigid Ultraâ€microporous Metal Organic Framework.. Chemistry - A European Journal, 2021, 27, 9446-9453.	3.3	20
18	Scalable Room-Temperature Synthesis of Highly Robust Ethane-Selective Metalâ€“Organic Frameworks for Efficient Ethylene Purification. Journal of the American Chemical Society, 2021, 143, 8654-8660.	13.7	124

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19	Indiumâ€“Organic Framework with soc Topology as a Versatile Catalyst for Highly Efficient One-Pot Strecker Synthesis of Î±-aminonitriles. ACS Applied Materials & Interfaces, 2021, 13, 52023-52033.	8.0	28
20	Toward an Understanding of the Propensity for Crystalline Hydrate Formation by Molecular Compounds. Part 2. Crystal Growth and Design, 2021, 21, 4927-4939.	3.0	13
21	Benchmark Acetylene Binding Affinity and Separation through Induced Fit in a Flexible Hybrid Ultramicroporous Material. Angewandte Chemie, 2021, 133, 20546-20553.	2.0	14
22	Breaking the trade-off between selectivity and adsorption capacity for gas separation. CheM, 2021, 7, 3085-3098.	11.7	68
23	Benchmark Acetylene Binding Affinity and Separation through Induced Fit in a Flexible Hybrid Ultramicroporous Material. Angewandte Chemie - International Edition, 2021, 60, 20383-20390.	13.8	56
24	Efficient propyne/propadiene separation by microporous crystalline physiadsorbents. Nature Communications, 2021, 12, 5768.	12.8	26
25	Pore Engineering for One-Step Ethylene Purification from a Three-Component Hydrocarbon Mixture. Journal of the American Chemical Society, 2021, 143, 1485-1492.	13.7	143
26	One-step ethylene production from a four-component gas mixture by a single physisorbent. Nature Communications, 2021, 12, 6507.	12.8	64
27	Tuning the Selectivity between C2H2 and CO2 in Molecular Porous Materials. Langmuir, 2021, 37, 13838-13845.	3.5	9
28	Simulations of H₂ Sorption in an Anthracene-Functionalized rht-Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2020, 124, 13753-13764.	3.1	1
29	Radiation-resistant metal-organic framework enables efficient separation of krypton fission gas from spent nuclear fuel. Nature Communications, 2020, 11, 3103.	12.8	54
30	Insights into the Gas Adsorption Mechanisms in Metalâ€“Organic Frameworks from Classical Molecular Simulations. Topics in Current Chemistry, 2020, 378, 14.	5.8	16
31	Insights into the Gas Adsorption Mechanisms in Metalâ€“Organic Frameworks from Classical Molecular Simulations. Topics in Current Chemistry Collections, 2020, , 215-279.	0.5	2
32	MPMC and MCMD: Free Highâ€Performance Simulation Software for Atomistic Systems. Advanced Theory and Simulations, 2019, 2, 1900113.	2.8	8
33	Synergistic sorbent separation for one-step ethylene purification from a four-component mixture. Science, 2019, 366, 241-246.	12.6	360
34	A Metalâ€“Organic Framework Based Methane Nanoâ€trap for the Capture of Coalâ€Mine Methane. Angewandte Chemie, 2019, 131, 10244-10247.	2.0	28
35	Molecular Sieving and Direct Visualization of CO₂ in Binding Pockets of an Ultramicroporous Lanthanide Metalâ€“Organic Framework Platform. ACS Applied Materials & Interfaces, 2019, 11, 23192-23197.	8.0	26
36	Investigating CO₂ Sorption in SIFSIX-3-M (M = Fe, Co, Ni, Cu, Zn) through Computational Studies. Crystal Growth and Design, 2019, 19, 3732-3743.	3.0	35

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37	A Metalâ€“Organic Framework Based Methane Nanoâ€trap for the Capture of Coalâ€Mine Methane. Angewandte Chemie - International Edition, 2019, 58, 10138-10141.	13.8	181
38	Robust Microporous Metalâ€“Organic Frameworks for Highly Efficient and Simultaneous Removal of Propyne and Propadiene from Propylene. Angewandte Chemie, 2019, 131, 10315-10320.	2.0	16
39	Robust Microporous Metalâ€“Organic Frameworks for Highly Efficient and Simultaneous Removal of Propyne and Propadiene from Propylene. Angewandte Chemie - International Edition, 2019, 58, 10209-10214.	13.8	69
40	Highly selective CO₂ removal for one-step liquefied natural gas processing by physisorbents. Chemical Communications, 2019, 55, 3219-3222.	4.1	31
41	InnenrÃ¼cktitelbild: A Metalâ€“Organic Framework Based Methane Nanoâ€trap for the Capture of Coalâ€Mine Methane (Angew. Chem. 30/2019). Angewandte Chemie, 2019, 131, 10483-10483.	2.0	0
42	Reversible Switching between Highly Porous and Nonporous Phases of an Interpenetrated Diamondoid Coordination Network That Exhibits Gateâ€Opening at Methane Storage Pressures. Angewandte Chemie - International Edition, 2018, 57, 5684-5689.	13.8	161
43	Reversible Switching between Highly Porous and Nonporous Phases of an Interpenetrated Diamondoid Coordination Network That Exhibits Gateâ€Opening at Methane Storage Pressures. Angewandte Chemie, 2018, 130, 5786-5791.	2.0	27
44	Efficient CO₂ Removal for Ultraâ€Pure CO Production by Two Hybrid Ultramicroporous Materials. Angewandte Chemie - International Edition, 2018, 57, 3332-3336.	13.8	52
45	Efficient CO₂ Removal for Ultraâ€Pure CO Production by Two Hybrid Ultramicroporous Materials. Angewandte Chemie, 2018, 130, 3390-3394.	2.0	12
46	Simulations of hydrogen, carbon dioxide, and small hydrocarbon sorption in a nitrogen-rich rht-metalâ€“organic framework. Physical Chemistry Chemical Physics, 2018, 20, 1761-1777.	2.8	15
47	Readily accessible shape-memory effect in a porous interpenetrated coordination network. Science Advances, 2018, 4, eaaq1636.	10.3	61
48	Impact of partial interpenetration in a hybrid ultramicroporous material on C₂H₂/C₂H₄ separation performance. Chemical Communications, 2018, 54, 3488-3491.	4.1	38
49	Investigating the Effects of Linker Extension on H₂ Sorption in the rht-Metalâ€“Organic Framework NU-111 by Molecular Simulations. Crystal Growth and Design, 2018, 18, 7599-7610.	3.0	9
50	Robust Ultramicroporous Metalâ€“Organic Frameworks with Benchmark Affinity for Acetylene. Angewandte Chemie, 2018, 130, 11137-11141.	2.0	85
51	Robust Ultramicroporous Metalâ€“Organic Frameworks with Benchmark Affinity for Acetylene. Angewandte Chemie - International Edition, 2018, 57, 10971-10975.	13.8	365
52	Investigating C₂H₂ Sorption in Î±-[M₃(O₂CH)₆] (M = Mg, Mn) Through Theoretical Studies. Crystal Growth and Design, 2018, 18, 5342-5352.	3.0	2
53	Hydrogen Adsorption in a Zeolitic Imidazolate Framework with lta Topology. Journal of Physical Chemistry C, 2018, 122, 15435-15445.	3.1	17
54	Theoretical study of the effect of halogen substitution in molecular porous materials for CO₂ and C₂H₂ sorption. AIMS Materials Science, 2018, 5, 226-245.	1.4	1

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55	Highly Selective Separation of C₂H₂ from CO₂ by a New Dichromate-Based Hybrid Ultramicroporous Material. ACS Applied Materials & Interfaces, 2017, 9, 33395-33400.	8.0	116
56	Partially Interpenetrated NbO Topology Metalâ€“Organic Framework Exhibiting Selective Gas Adsorption. Crystal Growth and Design, 2017, 17, 2711-2717.	3.0	30
57	The rotational dynamics of H₂ adsorbed in covalent organic frameworks. Physical Chemistry Chemical Physics, 2017, 19, 13075-13082.	2.8	17
58	Predictive models of gas sorption in a metalâ€“organic framework with open-metal sites and small pore sizes. Physical Chemistry Chemical Physics, 2017, 19, 18587-18602.	2.8	24
59	Comparing the mechanism and energetics of CO₂ sorption in the SIFSIX series. CrystEngComm, 2017, 19, 3338-3347.	2.6	22
60	High H₂ Sorption Energetics in Zeolitic Imidazolate Frameworks. Journal of Physical Chemistry C, 2017, 121, 1723-1733.	3.1	13
61	Effect of ring rotation upon gas adsorption in SIFSIX-3-M (M = Fe, Ni) pillared square grid networks. Chemical Science, 2017, 8, 2373-2380.	7.4	121
62	The effect of centred versus offset interpenetration on C₂H₂ sorption in hybrid ultramicroporous materials. Chemical Communications, 2017, 53, 11592-11595.	4.1	40
63	Investigating gas sorption in an rht-metalâ€“organic framework with 1,2,3-triazole groups. Physical Chemistry Chemical Physics, 2017, 19, 29204-29221.	2.8	8
64	Experimental and theoretical investigations of the gas adsorption sites in rht-metalâ€“organic frameworks. CrystEngComm, 2017, 19, 4646-4665.	2.6	20
65	Fine Tuning of MOFâ€505 Analogues To Reduce Lowâ€Pressure Methane Uptake and Enhance Methane Working Capacity. Angewandte Chemie, 2017, 129, 11584-11588.	2.0	33
66	Fine Tuning of MOFâ€505 Analogues To Reduce Lowâ€Pressure Methane Uptake and Enhance Methane Working Capacity. Angewandte Chemie - International Edition, 2017, 56, 11426-11430.	13.8	119
67	An unusual H2 sorption mechanism in PCN-14: insights from molecular simulation. Physical Chemistry Chemical Physics, 2016, 18, 21421-21430.	2.8	11
68	Hybrid Ultraâ€Microporous Materials for Selective Xenon Adsorption and Separation. Angewandte Chemie, 2016, 128, 8425-8429.	2.0	38
69	Hybrid Ultraâ€Microporous Materials for Selective Xenon Adsorption and Separation. Angewandte Chemie - International Edition, 2016, 55, 8285-8289.	13.8	137
70	Benchmark C2H2/CO2 and CO2/C2H2 Separation by Two Closely Related Hybrid Ultramicroporous Materials. CheM, 2016, 1, 753-765.	11.7	349
71	Towards an understanding of the propensity for crystalline hydrate formation by molecular compounds. IUCrJ, 2016, 3, 430-439.	2.2	49
72	Crystal engineering of a family of hybrid ultramicroporous materials based upon interpenetration and dichromate linkers. Chemical Science, 2016, 7, 5470-5476.	7.4	66

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73	Dynamics of H2 adsorbed in porous materials as revealed by computational analysis of inelastic neutron scattering spectra. Physical Chemistry Chemical Physics, 2016, 18, 17141-17158.	2.8	23
74	Accurate H₂ Sorption Modeling in the rht-MOF NOTT-112 Using Explicit Polarization. Crystal Growth and Design, 2016, 16, 6024-6032.	3.0	17
75	Tuning Pore Size in Squareâ€Lattice Coordination Networks for Sizeâ€Selective Sieving of CO₂. Angewandte Chemie, 2016, 128, 10424-10428.	2.0	43
76	Tuning Pore Size in Squareâ€Lattice Coordination Networks for Sizeâ€Selective Sieving of CO₂. Angewandte Chemie - International Edition, 2016, 55, 10268-10272.	13.8	237
77	Theoretical Investigations of CO₂ and H₂ Sorption in Robust Molecular Porous Materials. Langmuir, 2016, 32, 11492-11505.	3.5	17
78	A Robust Metal-Metalloporphyrin Framework Based upon a Secondary Building Unit of Infinite Nickel Oxide Chain. Crystal Growth and Design, 2016, 16, 1005-1009.	3.0	14
79	Dramatic Effect of the Electrostatic Parameters on H2 Sorption in an M-MOF-74 Analogue. Crystal Growth and Design, 2016, 16, 867-874.	3.0	23
80	Crystal Engineering of a 4,6-c fsc Platform That Can Serve as a Carbon Dioxide Single-Molecule Trap. Crystal Growth and Design, 2016, 16, 1071-1080.	3.0	21
81	Exceptional H₂ sorption characteristics in a Mg²⁺-based metalâ€“organic framework with small pores: insights from experimental and theoretical studies. Physical Chemistry Chemical Physics, 2016, 18, 1786-1796.	2.8	24
82	Theoretical Insights into the Tuning of Metal Binding Sites of Paddlewheels in rhtâ€Metalâ€“Organic Frameworks. ChemPhysChem, 2015, 16, 3170-3179.	2.1	14
83	Understanding Hydrogen Sorption in In-soc-MOF: A Charged Metal-Organic Framework with Open-Metal Sites, Narrow Channels, and Counterions. Crystal Growth and Design, 2015, 15, 1460-1471.	3.0	32
84	Remote Stabilization of Copper Paddlewheel Based Molecular Building Blocks in Metalâ€“Organic Frameworks. Chemistry of Materials, 2015, 27, 2144-2151.	6.7	72
85	Investigating H2Sorption in a Fluorinated Metalâ€“Organic Framework with Small Pores Through Molecular Simulation and Inelastic Neutron Scattering. Langmuir, 2015, 31, 7328-7336.	3.5	26
86	The local electric field favours more than exposed nitrogen atoms on CO₂ capture: a case study on the rht-type MOF platform. Chemical Communications, 2015, 51, 9636-9639.	4.1	48
87	Inelastic Neutron Scattering and Theoretical Studies of H2Sorption in a Dy(III)-Based Phosphine Coordination Material. Chemistry of Materials, 2015, 27, 7619-7626.	6.7	10
88	Novel mode of 2-fold interpenetration observed in a primitive cubic network of formula [Ni(1,2-bis(4-pyridyl)acetylene)₂(Cr₂O₇)]_n. Chemical Communications, 2015, 51, 14832-14835.	4.1	47
89	Hydrophobic pillared square grids for selective removal of CO₂ from simulated flue gas. Chemical Communications, 2015, 51, 15530-15533.	4.1	115
90	Understanding the H₂ Sorption Trends in the M-MOF-74 Series (M = Mg, Ni, Co, Zn). Journal of Physical Chemistry C, 2015, 119, 1078-1090.	3.1	84

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91	Investigating the Gas Sorption Mechanism in an rht-Metalâ€“Organic Framework through Computational Studies. Journal of Physical Chemistry C, 2014, 118, 439-456.	3.1	40
92	Modeling PCN-61 and PCN-66: Isostructural rht-Metalâ€“Organic Frameworks with Distinct CO₂ Sorption Mechanisms. Crystal Growth and Design, 2014, 14, 5599-5607.	3.0	23
93	A high rotational barrier for physisorbed hydrogen in an fcu-metalâ€“organic framework. Chemical Communications, 2014, 50, 14109-14112.	4.1	28
94	Simulations of hydrogen sorption in rht-MOF-1: identifying the binding sites through explicit polarization and quantum rotation calculations. Journal of Materials Chemistry A, 2014, 2, 2088-2100.	10.3	55
95	Dramatic effect of pore size reduction on the dynamics of hydrogen adsorbed in metalâ€“organic materials. Journal of Materials Chemistry A, 2014, 2, 13884.	10.3	27
96	Theoretical Investigations of CO₂ and CH₄ Sorption in an Interpenetrated Diamondoid Metalâ€“Organic Material. Langmuir, 2014, 30, 6454-6462.	3.5	35
97	Capturing the H₂â€“Metal Interaction in Mg-MOF-74 Using Classical Polarization. Journal of Physical Chemistry C, 2014, 118, 22683-22690.	3.1	40
98	Insights into an intriguing gas sorption mechanism in a polar metalâ€“organic framework with open-metal sites and narrow channels. Chemical Communications, 2014, 50, 7283-7286.	4.1	16
99	Introduction of Ï€-Complexation into Porous Aromatic Framework for Highly Selective Adsorption of Ethylene over Ethane. Journal of the American Chemical Society, 2014, 136, 8654-8660.	13.7	383
100	Putting the Squeeze on CH₄ and CO₂ through Control over Interpenetration in Diamondoid Nets. Journal of the American Chemical Society, 2014, 136, 5072-5077.	13.7	106
101	A Robust Molecular Porous Material with High CO₂ Uptake and Selectivity. Journal of the American Chemical Society, 2013, 135, 10950-10953.	13.7	236
102	Pillar substitution modulates CO2 affinity in â€œmmoâ€•topology networks. Chemical Communications, 2013, 49, 9809.	4.1	47
103	Enhancement of CO2 selectivity in a pillared pcu MOM platform through pillar substitution. Chemical Communications, 2013, 49, 1606.	4.1	87
104	Porous materials with optimal adsorption thermodynamics and kinetics for CO2 separation. Nature, 2013, 495, 80-84.	27.8	2,005
105	Understanding Hydrogen Sorption in a Metalâ€“Organic Framework with Open-Metal Sites and Amide Functional Groups. Journal of Physical Chemistry C, 2013, 117, 9340-9354.	3.1	74
106	Theoretical Investigations of CO₂ and H₂ Sorption in an Interpenetrated Square-Pillared Metalâ€“Organic Material. Journal of Physical Chemistry C, 2013, 117, 9970-9982.	3.1	36
107	Computational Studies of CO₂ Sorption and Separation in an Ultramicroporous Metalâ€“Organic Material. Journal of Physical Chemistry C, 2013, 117, 17687-17698.	3.1	45
108	Examining the Effects of Different Ring Configurations and Equatorial Fluorine Atom Positions on CO₂ Sorption in [Cu(bpy)₂SiF₆]. Crystal Growth and Design, 2013, 13, 4542-4548.	3.0	17

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109	A Polarizable and Transferable PHAST CO₂ Potential for Materials Simulation. Journal of Chemical Theory and Computation, 2013, 9, 5421-5429.	5.3	39
110	Efficient calculation of many-body induced electrostatics in molecular systems. Journal of Chemical Physics, 2013, 139, 184112.	3.0	32
111	Simulation of the Mechanism of Gas Sorption in a Metalâ€“Organic Framework with Open Metal Sites: Molecular Hydrogen in PCN-61. Journal of Physical Chemistry C, 2012, 116, 15538-15549.	3.1	76
112	Highly Selective CO₂ Uptake in Uninodal 6-Connected â€œmmoâ€•Nets Based upon MO₄^{2â€“} (M = Cr, Mo) Pillars. Journal of the American Chemical Society, 2012, 134, 19556-19559.	13.7	110