Berend Smit

List of Publications by Year in Descending Order

349 papers	30,962 citations	91 h-index	165 g-index
384 ext. papers	34,768 ext. citations	9.1 avg, IF	7.54 L-index

#	Paper	IF	Citations
349	Making Molecules Vibrate: Interactive Web Environment for the Teaching of Infrared Spectroscopy. *Journal of Chemical Education*, **2022**, 99, 561-569	2.4	3
348	Making the collective knowledge of chemistry open and machine actionable.. *Nature Chemistry*, **2022**, 14, 365-376	17.6	2
347	Characterization of Chemisorbed Species and Active Adsorption Sites in Mg-Al Mixed Metal Oxides for High-Temperature CO Capture.. *Chemistry of Materials*, **2022**, 34, 3893-3901	9.6	1
346	Toward Optimal Photocatalytic Hydrogen Generation from Water Using Pyrene-Based Metal-Organic Frameworks. *ACS Applied Materials & Interfaces*, **2021**, 13, 57118-57131	9.5	1
345	Buffered Coordination Modulation as a Means of Controlling Crystal Morphology and Molecular Diffusion in an Anisotropic Metal-Organic Framework. *Journal of the American Chemical Society*, **2021**, 143, 5044-5052	16.4	8
344	Enhanced Visible-Light-Driven Hydrogen Production through MOF/MOF Heterojunctions. *ACS Applied Materials & Interfaces*, **2021**, 13, 14239-14247	9.5	20
343	Multilevel screening of computation-ready, experimental metal-organic frameworks for natural gas purification. *AICHE Journal*, **2021**, 67, e17279	3.6	2
342	Toward smart carbon capture with machine learning. *Cell Reports Physical Science*, **2021**, 2, 100396	6.1	11
341	Bias free multiobjective active learning for materials design and discovery. *Nature Communications*, **2021**, 12, 2312	17.4	21
340	Pyrene-based metal organic frameworks: from synthesis to applications. *Chemical Society Reviews*, **2021**, 50, 3143-3177	58.5	28
339	AiiDAlab an ecosystem for developing, executing, and sharing scientific workflows. *Computational Materials Science*, **2021**, 188, 110165	3.2	18
338	Using collective knowledge to assign oxidation states of metal cations in metal-organic frameworks. *Nature Chemistry*, **2021**, 13, 771-777	17.6	12
337	Common workflows for computing material properties using different quantum engines. *Npj Computational Materials*, **2021**, 7,	10.9	4
336	Diversifying Databases of Metal Organic Frameworks for High-Throughput Computational Screening.. *ACS Applied Materials & Interfaces*, **2021**, 13, 61004-61014	9.5	4
335	A novel integrated Cr(VI) adsorption–photoreduction system using MOF@polymer composite beads. *Journal of Materials Chemistry A*, **2020**, 8, 9629-9637	13	30
334	Big-Data Science in Porous Materials: Materials Genomics and Machine Learning. *Chemical Reviews*, **2020**, 120, 8066-8129	68.1	128
333	Sustainable Hydrogenation of Nitroarenes to Anilines with Highly Active in-situ Generated Copper Nanoparticles. *ChemCatChem*, **2020**, 12, 2833-2839	5.2	6

332	Taking lanthanides out of isolation: tuning the optical properties of metal-organic frameworks. *Chemical Science*, **2020**, 11, 4164-4170	9.4	6
331	In Silico Discovery of Covalent Organic Frameworks for Carbon Capture. *ACS Applied Materials & Interfaces*, **2020**, 12, 21559-21568	9.5	27
330	Energy-based descriptors for photo-catalytically active metal□organic framework discovery. *Journal of Materials Chemistry A*, **2020**, 8, 4473-4482	13	14
329	Metal-organic frameworks as kinetic modulators for branched selectivity in hydroformylation. *Nature Communications*, **2020**, 11, 1059	17.4	23
328	On the Electronic and Optical Properties of Metal□Organic Frameworks: Case Study of MIL-125 and MIL-125-NH2. *Journal of Physical Chemistry C*, **2020**, 124, 4065-4072	3.8	26
327	Geometric landscapes for material discovery within energy-structure-function maps. *Chemical Science*, **2020**, 11, 5423-5433	9.4	12
326	Too Many Materials and Too Many Applications: An Experimental Problem Waiting for a Computational Solution. *ACS Central Science*, **2020**, 6, 1890-1900	16.8	28
325	The Role of Machine Learning in the Understanding and Design of Materials. *Journal of the American Chemical Society*, **2020**,	16.4	64
324	Understanding the diversity of the metal-organic framework ecosystem. *Nature Communications*, **2020**, 11, 4068	17.4	92
323	Thermoelasticity of Flexible Organic Crystals from Quasi-harmonic Lattice Dynamics: The Case of Copper(II) Acetylacetonate. *Journal of Physical Chemistry Letters*, **2020**, 11, 8543-8548	6.4	7
322	From Isolated Porphyrin Ligands to Periodic Al-PMOF: A Comparative Study of the Optical Properties Using DFT/TDDFT. *Journal of Physical Chemistry C*, **2020**, 124, 21751-21760	3.8	5
321	Materials Cloud, a platform for open computational science. *Scientific Data*, **2020**, 7, 299	8.2	70
320	Charge Separation and Charge Carrier Mobility in Photocatalytic Metal-Organic Frameworks. *Advanced Functional Materials*, **2020**, 30, 2003792	15.6	25
319	Optical absorption properties of metal-organic frameworks: solid state molecular perspective. *Physical Chemistry Chemical Physics*, **2020**, 22, 19512-19521	3.6	8
318	Insights into the Electronic Properties and Charge Transfer Mechanism of a Porphyrin Ruthenium-Based Metal□Organic Framework. *Chemistry of Materials*, **2020**, 32, 4194-4204	9.6	16
317	A data-driven perspective on the colours of metal-organic frameworks. *Chemical Science*, **2020**, 12, 3587-3598	9.4	7
316	Can Metal-Organic Frameworks Be Used for Cannabis Breathalyzers?. *ACS Applied Materials & Interfaces*, **2019**, 11, 34777-34786	9.5	1
315	Applicability of Tail Corrections in the Molecular Simulations of Porous Materials. *Journal of Chemical Theory and Computation*, **2019**, 15, 5635-5641	6.4	14

314	Simulating Enhanced Methane Deliverable Capacity of Guest Responsive Pores in Intrinsically Flexible MOFs. *Journal of Physical Chemistry Letters*, **2019**, 10, 5929-5934	6.4	13
313	Building a Consistent and Reproducible Database for Adsorption Evaluation in Covalent-Organic Frameworks. *ACS Central Science*, **2019**, 5, 1663-1675	16.8	49
312	Capturing chemical intuition in synthesis of metal-organic frameworks. *Nature Communications*, **2019**, 10, 539	17.4	92
311	Ab Initio Flexible Force Field for Metal-Organic Frameworks Using Dummy Model Coordination Bonds. *Journal of Chemical Theory and Computation*, **2019**, 15, 3666-3677	6.4	5
310	Combined Nuclear Magnetic Resonance and Molecular Dynamics Study of Methane Adsorption in M2(dobdc) Metal□Organic Frameworks. *Journal of Physical Chemistry C*, **2019**, 123, 12286-12295	3.8	7
309	DORI Reveals the Influence of Noncovalent Interactions on Covalent Bonding Patterns in Molecular Crystals Under Pressure. *Journal of Physical Chemistry Letters*, **2019**, 10, 1482-1488	6.4	9
308	Metal Substitution as the Method of Modifying Electronic Structure of Metal-Organic Frameworks. *Journal of the American Chemical Society*, **2019**, 141, 6271-6278	16.4	73
307	Nucleobase pairing and photodimerization in a biologically derived metal-organic framework nanoreactor. *Nature Communications*, **2019**, 10, 1612	17.4	31
306	Pushing the limit of Cs incorporation into FAPbBr3 perovskite to enhance solar cells performances. *APL Materials*, **2019**, 7, 041110	5.7	21
305	Sim-to-real transfer reinforcement learning for control of thermal effects of an atmospheric pressure plasma jet. *Plasma Sources Science and Technology*, **2019**, 28, 095019	3.5	16
304	Preserving Porosity of Mesoporous Metal-Organic Frameworks through the Introduction of Polymer Guests. *Journal of the American Chemical Society*, **2019**, 141, 12397-12405	16.4	40
303	Guest-dependent negative thermal expansion in a lanthanide-based metal□organic framework. *CrystEngComm*, **2019**, 21, 5292-5298	3.3	1
302	Automated Multiscale Approach To Predict Self-Diffusion from a Potential Energy Field. *Journal of Chemical Theory and Computation*, **2019**, 15, 2127-2141	6.4	16
301	Amine Dynamics in Diamine-Appended Mg(dobpdc) Metal-Organic Frameworks. *Journal of Physical Chemistry Letters*, **2019**, 10, 7044-7049	6.4	10
300	Carbons with Regular Pore Geometry Yield Fundamental Insights into Supercapacitor Charge Storage. *ACS Central Science*, **2019**, 5, 1813-1823	16.8	28
299	Data-driven design of metal-organic frameworks for wet flue gas CO capture. *Nature*, **2019**, 576, 253-256	50.4	192
298	Evaluating Charge Equilibration Methods To Generate Electrostatic Fields in Nanoporous Materials. *Journal of Chemical Theory and Computation*, **2019**, 15, 382-401	6.4	33
297	Distinguishing Metal-Organic Frameworks. *Crystal Growth and Design*, **2018**, 18, 1738-1747	3.5	53

296	Shedding Light on the Protonation States and Location of Protonated N Atoms of Adenine in Metal-Organic Frameworks. *Inorganic Chemistry*, **2018**, 57, 1888-1900	5.1	16
295	Cutting Materials in Half: A Graph Theory Approach for Generating Crystal Surfaces and Its Prediction of 2D Zeolites. *ACS Central Science*, **2018**, 4, 235-245	16.8	31
294	Photocatalytic hydrogen generation from a visible-light responsive metal□organic framework system: the impact of nickel phosphide nanoparticles. *Journal of Materials Chemistry A*, **2018**, 6, 2476-2481	13	68
293	Unexpected Diffusion Anisotropy of Carbon Dioxide in the Metal-Organic Framework Zn(dobpdc). *Journal of the American Chemical Society*, **2018**, 140, 1663-1673	16.4	42
292	Lanthanide-based near-infrared emitting metal-organic frameworks with tunable excitation wavelengths and high quantum yields. *Chemical Communications*, **2018**, 54, 6816-6819	5.8	18
291	Carbon capture and storage (CCS): the way forward. *Energy and Environmental Science*, **2018**, 11, 1062-1176	35.4	1368
290	Metal-Organic Framework Beads: Porous Metal□Organic Framework@Polymer Beads for Iodine Capture and Recovery Using a Gas-Sparged Column (Adv. Funct. Mater. 30/2018). *Advanced Functional Materials*, **2018**, 28, 1870211	15.6	3
289	Anomalous Effects of Velocity Rescaling Algorithms: The Flying Ice Cube Effect Revisited. *Journal of Chemical Theory and Computation*, **2018**, 14, 5262-5272	6.4	42
288	High-Throughput Screening Approach for Nanoporous Materials Genome Using Topological Data Analysis: Application to Zeolites. *Journal of Chemical Theory and Computation*, **2018**, 14, 4427-4437	6.4	35
287	Generating carbon schwarzites via zeolite-templating. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, E8116-E8124	11.5	54
286	Photocatalytic Hydrogen Generation from a Visible-Light-Responsive Metal-Organic Framework System: Stability versus Activity of Molybdenum Sulfide Cocatalysts. *ACS Applied Materials & Interfaces*, **2018**, 10, 30035-30039	9.5	51
285	Porous Metal□Organic Framework@Polymer Beads for Iodine Capture and Recovery Using a Gas-Sparged Column. *Advanced Functional Materials*, **2018**, 28, 1801596	15.6	73
284	In Silico Design of 2D and 3D Covalent Organic Frameworks for Methane Storage Applications. *Chemistry of Materials*, **2018**, 30, 5069-5086	9.6	57
283	Improving the Mechanical Stability of Metal-Organic Frameworks Using Chemical Caryatids. *ACS Central Science*, **2018**, 4, 832-839	16.8	43
282	Text Mining Metal-Organic Framework Papers. *Journal of Chemical Information and Modeling*, **2018**, 58, 244-251	6.1	26
281	Dual-Functional Photocatalysis: Concurrent Photocatalytic Hydrogen Generation and Dye Degradation Using MIL-125-NH2 under Visible Light Irradiation (Adv. Funct. Mater. 52/2018). *Advanced Functional Materials*, **2018**, 28, 1870373	15.6	4
280	Biporous Metal-Organic Framework with Tunable CO/CH Separation Performance Facilitated by Intrinsic Flexibility. *ACS Applied Materials & Interfaces*, **2018**, 10, 36144-36156	9.5	26
279	Concurrent Photocatalytic Hydrogen Generation and Dye Degradation Using MIL-125-NH2 under Visible Light Irradiation. *Advanced Functional Materials*, **2018**, 28, 1806368	15.6	71

278	Flat-Histogram Monte Carlo as an Efficient Tool To Evaluate Adsorption Processes Involving Rigid and Deformable Molecules. *Journal of Chemical Theory and Computation*, **2018**, 14, 6149-6158	6.4	10
277	Impact of the strength and spatial distribution of adsorption sites on methane deliverable capacity in nanoporous materials. *Chemical Engineering Science*, **2017**, 159, 18-30	4.4	23
276	Statistical mechanical model of gas adsorption in porous crystals with dynamic moieties. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E287-E296	11.5	29
275	Rational Design of a Low-Cost, High-Performance Metal-Organic Framework for Hydrogen Storage and Carbon Capture. *Journal of Physical Chemistry C*, **2017**, 121, 1171-1181	3.8	60
274	Adsorbate-induced lattice deformation in IRMOF-74 series. *Nature Communications*, **2017**, 8, 13945	17.4	23
273	Materials Genome in Action: Identifying the Performance Limits of Physical Hydrogen Storage. *Chemistry of Materials*, **2017**, 29, 2844-2854	9.6	123
272	Performance of van der Waals Corrected Functionals for Guest Adsorption in the M(dobdc) Metal-Organic Frameworks. *Journal of Physical Chemistry A*, **2017**, 121, 4139-4151	2.8	32
271	Predicting Product Distribution of Propene Dimerization in Nanoporous Materials. *ACS Catalysis*, **2017**, 7, 3940-3948	13.1	4
270	Formation pathways of metal□organic frameworks proceeding through partial dissolution of the metastable phase. *CrystEngComm*, **2017**, 19, 3407-3413	3.3	12
269	Translational and Rotational Motion of C8 Aromatics Adsorbed in Isotropic Porous Media (MOF-5): NMR Studies and MD Simulations. *Journal of Physical Chemistry C*, **2017**, 121, 15456-15462	3.8	18
268	Quantifying similarity of pore-geometry in nanoporous materials. *Nature Communications*, **2017**, 8, 15396	17.4	66
267	The Influence of Intrinsic Framework Flexibility on Adsorption in Nanoporous Materials. *Journal of the American Chemical Society*, **2017**, 139, 5547-5557	16.4	82
266	Mixed-linker UiO-66: structure-property relationships revealed by a combination of high-resolution powder X-ray diffraction and density functional theory calculations. *Physical Chemistry Chemical Physics*, **2017**, 19, 1551-1559	3.6	35
265	Force-Field Prediction of Materials Properties in Metal-Organic Frameworks. *Journal of Physical Chemistry Letters*, **2017**, 8, 357-363	6.4	100
264	Effects of Pore and Cage Topology on the Thermodynamics of n-Alkane Adsorption at Br□sted Protons in Zeolites at High Temperature. *Journal of Physical Chemistry C*, **2017**, 121, 1618-1638	3.8	12
263	Uncovering the Local Magnesium Environment in the Metal□Organic Framework Mg2(dobpdc) Using 25Mg NMR Spectroscopy. *Journal of Physical Chemistry C*, **2017**, 121, 19938-19945	3.8	13
262	Metal-Organic Frameworks Invert Molecular Reactivity: Lewis Acidic Phosphonium Zwitterions Catalyze the Aldol-Tishchenko Reaction. *Journal of the American Chemical Society*, **2017**, 139, 18166-18169	16.4	25
261	Accurate Characterization of the Pore Volume in Microporous Crystalline Materials. *Langmuir*, **2017**, 33, 14529-14538	4	99

260	Computational development of the nanoporous materials genome. *Nature Reviews Materials*, **2017**, 2,	73.3	84
259	Origin of the Strong Interaction between Polar Molecules and Copper(II) Paddle-Wheels in Metal Organic Frameworks. *Journal of Physical Chemistry C*, **2017**, 121, 15135-15144	3.8	15
258	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
257	CCS - A technology for now: general discussion. *Faraday Discussions*, **2016**, 192, 125-151	3.6	4
256	CCS - A technology for the future: general discussion. *Faraday Discussions*, **2016**, 192, 303-335	3.6	2
255	Effects of Zeolite Structural Confinement on Adsorption Thermodynamics and Reaction Kinetics for Monomolecular Cracking and Dehydrogenation of n-Butane. *Journal of the American Chemical Society*, **2016**, 138, 4739-56	16.4	53
254	pyIAST: Ideal adsorbed solution theory (IAST) Python package. *Computer Physics Communications*, **2016**, 200, 364-380	4.2	115
253	Pre-transition effects mediate forces of assembly between transmembrane proteins. *ELife*, **2016**, 5, e13150	8.9	48
252	Author response: Pre-transition effects mediate forces of assembly between transmembrane proteins **2016**,		2
251	Metal-organic framework with optimally selective xenon adsorption and separation. *Nature Communications*, **2016**, 7, ncomms11831	17.4	232
250	design and screening of hypothetical MOF-74 analogs and their experimental synthesis. *Chemical Science*, **2016**, 7, 6263-6272	9.4	50
249	Carbon Capture and Storage: introductory lecture. *Faraday Discussions*, **2016**, 192, 9-25	3.6	30
248	First-principles Hubbard U approach for small molecule binding in metal-organic frameworks. *Journal of Chemical Physics*, **2016**, 144, 174104	3.9	47
247	Force Field Development from Periodic Density Functional Theory Calculations for Gas Separation Applications Using Metal□Organic Frameworks. *Journal of Physical Chemistry C*, **2016**, 120, 12590-12604	3.8	71
246	Cutting the cost of carbon capture: a case for carbon capture and utilization. *Faraday Discussions*, **2016**, 192, 391-414	3.6	25
245	Small-Molecule Adsorption in Open-Site Metal□Organic Frameworks: A Systematic Density Functional Theory Study for Rational Design. *Chemistry of Materials*, **2015**, 27, 668-678	9.6	198
244	Cooperative insertion of CO2 in diamine-appended metal-organic frameworks. *Nature*, **2015**, 519, 303-8	50.4	807
243	CO induced phase transitions in diamine-appended metal-organic frameworks. *Chemical Science*, **2015**, 6, 5177-5185	9.4	42

242	Carbon capture turned upside down: high-temperature adsorption & low-temperature desorption (HALD). *Energy and Environmental Science*, **2015**, 8, 2480-2491	35.4	18
241	Systematic Tuning and Multifunctionalization of Covalent Organic Polymers for Enhanced Carbon Capture. *Journal of the American Chemical Society*, **2015**, 137, 13301-7	16.4	171
240	Critical Factors Driving the High Volumetric Uptake of Methane in Cu(btc). *Journal of the American Chemical Society*, **2015**, 137, 10816-25	16.4	61
239	In Silico Discovery of High Deliverable Capacity Metal-Organic Frameworks. *Journal of Physical Chemistry C*, **2015**, 119, 186-195	3.8	42
238	Nanoporous Materials Can Tune the Critical Point of a Pure Substance. *Angewandte Chemie - International Edition*, **2015**, 54, 14349-52	16.4	11
237	Understanding Small-Molecule Interactions in Metal-Organic Frameworks: Coupling Experiment with Theory. *Advanced Materials*, **2015**, 27, 5785-96	24	30
236	Computer-Aided Search for Materials to Store Natural Gas for Vehicles. *Frontiers for Young Minds*, **2015**, 3,	1.5	2
235	Adsorption Thermodynamics and Intrinsic Activation Parameters for Monomolecular Cracking of n-Alkanes on Brønsted Acid Sites in Zeolites. *Journal of Physical Chemistry C*, **2015**, 119, 10427-10438	3.8	42
234	What Are the Best Materials To Separate a Xenon/Krypton Mixture?. *Chemistry of Materials*, **2015**, 27, 4459-4475	9.6	156
233	Nanoporous Materials Can Tune the Critical Point of a Pure Substance. *Angewandte Chemie*, **2015**, 127, 14557-14560	3.6	5
232	Screening Materials Relevant for Energy Technologies. *Chimia*, **2015**, 69, 248-52	1.3	5
231	Water adsorption in metal-organic frameworks with open-metal sites. *AICHE Journal*, **2015**, 61, 677-687	3.6	34
230	The materials genome in action: identifying the performance limits for methane storage. *Energy and Environmental Science*, **2015**, 8, 1190-1199	35.4	263
229	PSII-LHCII supercomplex organizations in photosynthetic membrane by coarse-grained simulation. *Journal of Physical Chemistry B*, **2015**, 119, 3999-4008	3.4	11
228	Small scale membrane mechanics. *Biomechanics and Modeling in Mechanobiology*, **2014**, 13, 697-711	3.8	24
227	In silico design of porous polymer networks: high-throughput screening for methane storage materials. *Journal of the American Chemical Society*, **2014**, 136, 5006-22	16.4	125
226	Design of a metal-organic framework with enhanced back bonding for separation of N and CH. *Journal of the American Chemical Society*, **2014**, 136, 698-704	16.4	134
225	On the flexibility of metal-organic frameworks. *Journal of the American Chemical Society*, **2014**, 136, 2228-31	16.4	165

224	A hybrid absorption-adsorption method to efficiently capture carbon. *Nature Communications*, **2014**, 5, 5147	17.4	105
223	Toward a Materials Genome Approach for ionic liquids: synthesis guided by ab initio property maps. *Journal of Physical Chemistry B*, **2014**, 118, 13609-20	3.4	17
222	Optimizing nanoporous materials for gas storage. *Physical Chemistry Chemical Physics*, **2014**, 16, 5499-513	3.6	67
221	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
220	Evaluating different classes of porous materials for carbon capture. *Energy and Environmental Science*, **2014**, 7, 4132-4146	35.4	152
219	Comprehensive study of carbon dioxide adsorption in the metal□organic frameworks M2(dobdc) (M = Mg, Mn, Fe, Co, Ni, Cu, Zn). *Chemical Science*, **2014**, 5, 4569-4581	9.4	267
218	In Silico Design of Three-Dimensional Porous Covalent Organic Frameworks via Known Synthesis Routes and Commercially Available Species. *Journal of Physical Chemistry C*, **2014**, 118, 23790-23802	3.8	31
217	CO2 Adsorption in Fe2(dobdc): A Classical Force Field Parameterized from Quantum Mechanical Calculations. *Journal of Physical Chemistry C*, **2014**, 118, 12230-12240	3.8	40
216	Force-Field Development from Electronic Structure Calculations with Periodic Boundary Conditions: Applications to Gaseous Adsorption and Transport in Metal-Organic Frameworks. *Journal of Chemical Theory and Computation*, **2014**, 10, 1477-88	6.4	97
215	Reversible CO binding enables tunable CO/H□and CO/N□separations in metal-organic frameworks with exposed divalent metal cations. *Journal of the American Chemical Society*, **2014**, 136, 10752-61	16.4	160
214	Understanding Trends in CO2 Adsorption in Metal-Organic Frameworks with Open-Metal Sites. *Journal of Physical Chemistry Letters*, **2014**, 5, 861-5	6.4	113
213	Redox chemistry and metal-insulator transitions intertwined in a nano-porous material. *Nature Communications*, **2014**, 5, 4032	17.4	11
212	The Grand Challenges in Carbon Capture, Utilization, and Storage. *Frontiers in Energy Research*, **2014**, 2,	3.8	37
211	Kinetically tuned dimensional augmentation as a versatile synthetic route towards robust metal-organic frameworks. *Nature Communications*, **2014**, 5, 5723	17.4	258
210	Computational screening of porous metal-organic frameworks and zeolites for the removal of SO2 and NOx from flue gases. *AICHE Journal*, **2014**, 60, 2314-2323	3.6	89
209	Computational carbon capture **2014**,		2
208	Introduction to Carbon Capture and Sequestration **2014**,		83
207	Understanding the effect of side groups in ionic liquids on carbon-capture properties: a combined experimental and theoretical effort. *Physical Chemistry Chemical Physics*, **2013**, 15, 3264-72	3.6	26

206	Molecular simulation study of the competitive adsorption of H2O and CO2 in zeolite 13X. *Langmuir*, **2013**, 29, 15936-42	4	75
205	Mapping of functional groups in metal-organic frameworks. *Science*, **2013**, 341, 882-5	33.3	349
204	Modeling Methane Adsorption in Interpenetrating Porous Polymer Networks. *Journal of Physical Chemistry C*, **2013**, 117, 20037-20042	3.8	24
203	Lipid mediated packing of transmembrane helices a dissipative particle dynamics study. *Soft Matter*, **2013**, 9, 2673	3.6	14
202	Methane storage capabilities of diamond analogues. *Physical Chemistry Chemical Physics*, **2013**, 15, 20937-42	3.6	9
201	Evaluating mixture adsorption models using molecular simulation. *AICHE Journal*, **2013**, 59, 3054-3064	3.6	23
200	Understanding CO2 Dynamics in Metal Organic Frameworks with Open Metal Sites. *Angewandte Chemie*, **2013**, 125, 4506-4509	3.6	31
199	New materials for methane capture from dilute and medium-concentration sources. *Nature Communications*, **2013**, 4, 1694	17.4	84
198	Understanding CO2 dynamics in metal-organic frameworks with open metal sites. *Angewandte Chemie - International Edition*, **2013**, 52, 4410-3	16.4	143
197	On the Thermodynamics of Framework Breathing: A Free Energy Model for Gas Adsorption in MIL-53. *Journal of Physical Chemistry C*, **2013**, 117, 11540-11554	3.8	53
196	Large-scale screening of zeolite structures for CO2 membrane separations. *Journal of the American Chemical Society*, **2013**, 135, 7545-52	16.4	93
195	The mechanism of carbon dioxide adsorption in an alkylamine-functionalized metal-organic framework. *Journal of the American Chemical Society*, **2013**, 135, 7402-5	16.4	175
194	Mail-Order Metal Organic Frameworks (MOFs): Designing Isoreticular MOF-5 Analogues Comprising Commercially Available Organic Molecules. *Journal of Physical Chemistry C*, **2013**, 117, 12159-12167	3.8	60
193	Probing adsorption interactions in metal-organic frameworks using X-ray spectroscopy. *Journal of the American Chemical Society*, **2013**, 135, 18183-90	16.4	47
192	CO2 capture by metal-organic frameworks with van der Waals density functionals. *Journal of Physical Chemistry A*, **2012**, 116, 4957-64	2.8	86
191	Understanding the phase behavior of coarse-grained model lipid bilayers through computational calorimetry. *Journal of Physical Chemistry B*, **2012**, 116, 1551-69	3.4	62
190	On the Equivalence of Schemes for Simulating Bilayers at Constant Surface Tension. *Journal of Chemical Theory and Computation*, **2012**, 8, 404-17	6.4	4
189	Ligand-assisted enhancement of CO2 capture in metal-organic frameworks. *Journal of the American Chemical Society*, **2012**, 134, 6714-9	16.4	82

188	Monte Carlo Study on the Water Meniscus Condensation and Capillary Force in Atomic Force Microscopy. *Journal of Physical Chemistry C*, **2012**, 116, 21923-21931	3.8	33
187	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
186	High-Throughput Characterization of Porous Materials Using Graphics Processing Units. *Journal of Chemical Theory and Computation*, **2012**, 8, 1684-93	6.4	53
185	Predicting Local Transport Coefficients at Solid□Gas Interfaces. *Journal of Physical Chemistry C*, **2012**, 116, 18878-18883	3.8	31
184	Ab initio carbon capture in open-site metal-organic frameworks. *Nature Chemistry*, **2012**, 4, 810-6	17.6	263
183	Diffusion in confinement: kinetic simulations of self- and collective diffusion behavior of adsorbed gases. *Physical Chemistry Chemical Physics*, **2012**, 14, 11600-9	3.6	30
182	Similarity-driven discovery of zeolite materials for adsorption-based separations. *ChemPhysChem*, **2012**, 13, 3595-7	3.2	38
181	In silico screening of carbon-capture materials. *Nature Materials*, **2012**, 11, 633-41	27	433
180	Robust driving forces for transmembrane helix packing. *Biophysical Journal*, **2012**, 103, 1227-35	2.9	19
179	Combined Density Functional Theory and Monte Carlo Analysis of Monomolecular Cracking of Light Alkanes Over H-ZSM-5. *Journal of Physical Chemistry C*, **2012**, 116, 23408-23417	3.8	50
178	Large-scale computational screening of zeolites for ethane/ethene separation. *Langmuir*, **2012**, 28, 11914-9	4	74
177	Addressing challenges of identifying geometrically diverse sets of crystalline porous materials. *Journal of Chemical Information and Modeling*, **2012**, 52, 308-18	6.1	148
176	Efficient Monte Carlo Simulations of Gas Molecules Inside Porous Materials. *Journal of Chemical Theory and Computation*, **2012**, 8, 2336-43	6.4	31
175	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
174	Adsorption and diffusion in zeolites: the pitfall of isotypic crystal structures. *Molecular Simulation*, **2011**, 37, 986-989	2	13
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