Berend Smit

List of Publications by Citations

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	Carbon dioxide capture: prospects for new materials. *Angewandte Chemie - International Edition*, **2010**, 49, 6058-82	16.4	3035
348	Carbon capture and storage (CCS): the way forward. *Energy and Environmental Science*, **2018**, 11, 1062-1176	35.4	1368
347	Cooperative insertion of CO2 in diamine-appended metal-organic frameworks. *Nature*, **2015**, 519, 303-8	50.4	807
346	Understanding Molecular Simulation. *Computers in Physics*, **1997**, 11, 351		621
345	Molecular simulations of zeolites: adsorption, diffusion, and shape selectivity. *Chemical Reviews*, **2008**, 108, 4125-84	68.1	564
344	In silico screening of carbon-capture materials. *Nature Materials*, **2012**, 11, 633-41	27	433
343	Computer simulations of vapor□quid phase equilibria of n-alkanes. *Journal of Chemical Physics*, **1995**, 102, 2126-2140	3.9	423
342	Simulating the critical behaviour of complex fluids. *Nature*, **1993**, 365, 330-332	50.4	406
341	Metal-organic frameworks as adsorbents for hydrogen purification and precombustion carbon dioxide capture. *Journal of the American Chemical Society*, **2011**, 133, 5664-7	16.4	405
340	Selective binding of O2 over N2 in a redox-active metal-organic framework with open iron(II) coordination sites. *Journal of the American Chemical Society*, **2011**, 133, 14814-22	16.4	404
339	Towards a molecular understanding of shape selectivity. *Nature*, **2008**, 451, 671-8	50.4	403
338	Molecular Dynamics Simulations **2002**, 63-107		391
337	Novel scheme to study structural and thermal properties of continuously deformable molecules. *Journal of Physics Condensed Matter*, **1992**, 4, 3053-3076	1.8	356
336	Mapping of functional groups in metal-organic frameworks. *Science*, **2013**, 341, 882-5	33.3	349
335	Monte Carlo Simulations **2002**, 23-61		324
334	Effect of cholesterol on the structure of a phospholipid bilayer. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 3654-8	11.5	304
333	Why Clays Swell. *Journal of Physical Chemistry B*, **2002**, 106, 12664-12667	3.4	299

332	Computer simulations in the Gibbs ensemble. *Molecular Physics*, **1989**, 68, 931-950	1.7	286
331	United Atom Force Field for Alkanes in Nanoporous Materials. *Journal of Physical Chemistry B*, **2004**, 108, 12301-12313	3.4	282
330	Abscheidung von Kohlendioxid: Perspektiven für neue Materialien. *Angewandte Chemie*, **2010**, 122, 6194-6219	9.6	275
329	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
328	Chemie in cyberspace **1999**,		267
327	The materials genome in action: identifying the performance limits for methane storage. *Energy and Environmental Science*, **2015**, 8, 1190-1199	35.4	263
326	Ab initio carbon capture in open-site metal-organic frameworks. *Nature Chemistry*, **2012**, 4, 810-6	17.6	263
325	Kinetically tuned dimensional augmentation as a versatile synthetic route towards robust metal-organic frameworks. *Nature Communications*, **2014**, 5, 5723	17.4	258
324	Comparative molecular simulation study of CO2/N2 and CH4/N2 separation in zeolites and metal-organic frameworks. *Langmuir*, **2009**, 25, 5918-26	4	256
323	What makes a polar liquid a liquid?. *Physical Review Letters*, **1993**, 71, 3991-3994	7.4	253
322	Mesoscopic models of biological membranes. *Physics Reports*, **2006**, 437, 1-54	27.7	236
321	Metal-organic framework with optimally selective xenon adsorption and separation. *Nature Communications*, **2016**, 7, ncomms11831	17.4	232
320	Molecular Simulation Studies of Separation of CO2/N2, CO2/CH4, and CH4/N2 by ZIFs. *Journal of Physical Chemistry C*, **2010**, 114, 8515-8522	3.8	231
319	Understanding the role of sodium during adsorption: a force field for alkanes in sodium-exchanged faujasites. *Journal of the American Chemical Society*, **2004**, 126, 11377-86	16.4	222
318	Simulation studies of protein-induced bilayer deformations, and lipid-induced protein tilting, on a mesoscopic model for lipid bilayers with embedded proteins. *Biophysical Journal*, **2005**, 88, 1778-98	2.9	219
317	Commensurate 'freezing' of alkanes in the channels of a zeolite. *Nature*, **1995**, 374, 42-44	50.4	218
316	Lithium-doped 3D covalent organic frameworks: high-capacity hydrogen storage materials. *Angewandte Chemie - International Edition*, **2009**, 48, 4730-3	16.4	216
315	Computer Simulations of the Energetics and Siting of n-Alkanes in Zeolites. *The Journal of Physical Chemistry*, **1994**, 98, 8442-8452		203

314	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
313	Data-driven design of metal-organic frameworks for wet flue gas CO2 capture. *Nature*, **2019**, 576, 253-256	50.4	192
312	Doping of alkali, alkaline-earth, and transition metals in covalent-organic frameworks for enhancing CO2 capture by first-principles calculations and molecular simulations. *ACS Nano*, **2010**, 4, 4225-37	16.7	184
311	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
310	Entropy effects during sorption of alkanes in zeolites. *Chemical Society Reviews*, **2002**, 31, 185-94	58.5	174
309	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
308	On the flexibility of metal-organic frameworks. *Journal of the American Chemical Society*, **2014**, 136, 2228-31	16.4	165
307	Direct simulation of phase equilibria of chain molecules. *Journal of Physics Condensed Matter*, **1992**, 4, L255-L259	1.8	165
306	Phase behavior of model lipid bilayers. *Journal of Physical Chemistry B*, **2005**, 109, 6553-63	3.4	164
305	Calculation of the chemical potential in the Gibbs ensemble. *Molecular Physics*, **1989**, 68, 951-958	1.7	161
304	Reversible CO binding enables tunable CO/H2 and CO/N2 separations in metal-organic frameworks with exposed divalent metal cations. *Journal of the American Chemical Society*, **2014**, 136, 10752-61	16.4	160
303	What Are the Best Materials To Separate a Xenon/Krypton Mixture?. *Chemistry of Materials*, **2015**, 27, 4459-4475	9.6	156
302	Investigation of Surfactant Efficiency Using Dissipative Particle Dynamics. *Langmuir*, **2003**, 19, 8195-8205	4	155
301	Evaluating different classes of porous materials for carbon capture. *Energy and Environmental Science*, **2014**, 7, 4132-4146	35.4	152
300	Molecular Simulations of Swelling Clay Minerals. *Journal of Physical Chemistry B*, **2004**, 108, 7586-7596	3.4	150
299	Addressing challenges of identifying geometrically diverse sets of crystalline porous materials. *Journal of Chemical Information and Modeling*, **2012**, 52, 308-18	6.1	148
298	Computer simulations of surfactant self-assembly. *Langmuir*, **1993**, 9, 9-11	4	148
297	Adsorption of Linear and Branched Alkanes in the Zeolite Silicalite-1. *Journal of the American Chemical Society*, **1998**, 120, 5599-5600	16.4	145

296	Understanding CO2 dynamics in metal-organic frameworks with open metal sites. *Angewandte Chemie - International Edition*, **2013**, 52, 4410-3	16.4	143
295	Grand canonical Monte Carlo simulations of chain molecules: adsorption isotherms of alkanes in zeolites. *Molecular Physics*, **1995**, 85, 153-172	1.7	139
294	Hysteresis in clay swelling induced by hydrogen bonding: accurate prediction of swelling states. *Langmuir*, **2006**, 22, 1223-34	4	138
293	Molecular simulations of lipid-mediated protein-protein interactions. *Biophysical Journal*, **2008**, 95, 1851-65	3.9	136
292	Force field parametrization through fitting on inflection points in isotherms. *Physical Review Letters* , **2004**, 93, 088302	7.4	136
291	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
290	Big-Data Science in Porous Materials: Materials Genomics and Machine Learning. *Chemical Reviews*, **2020**, 120, 8066-8129	68.1	128
289	Molecular simulation of loading-dependent diffusion in nanoporous materials using extended dynamically corrected transition state theory. *Journal of Chemical Physics*, **2005**, 122, 224712	3.9	128
288	Phase Behavior and Induced Interdigitation in Bilayers Studied with Dissipative Particle Dynamics. *Journal of Physical Chemistry B*, **2003**, 107, 11491-11501	3.4	128
287	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
286	Materials Genome in Action: Identifying the Performance Limits of Physical Hydrogen Storage. *Chemistry of Materials*, **2017**, 29, 2844-2854	9.6	123
285	Molecular Simulation of the Vapor-Liquid Coexistence Curve of Methanol. *The Journal of Physical Chemistry*, **1995**, 99, 1831-1833		122
284	Simulating the Adsorption Isotherms of Methane, Ethane, and Propane in the Zeolite Silicalite. *The Journal of Physical Chemistry*, **1995**, 99, 5597-5603		120
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280	Molecular simulations in zeolitic process design. *Chemical Engineering Science*, **2003**, 58, 557-568	4.4	113
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272	Force-Field Prediction of Materials Properties in Metal-Organic Frameworks. *Journal of Physical Chemistry Letters*, **2017**, 8, 357-363	6.4	100
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268	Parallel Monte Carlo simulations. *Physical Review E*, **1995**, 51, 1560-1568	2.4	96
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258	CO2 capture by metal-organic frameworks with van der Waals density functionals. *Journal of Physical Chemistry A*, **2012**, 116, 4957-64	2.8	86
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207	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

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