Juergen Eckert

List of Publications by Year in descending order

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49 papers	7,800 citations	218662 26 h-index	197805 49 g-index
54 all docs	54 docs citations	54 times ranked	8222 citing authors

#	Article	IF	Citations
1	Hydrogen Storage in Microporous Metal-Organic Frameworks. Science, 2003, 300, 1127-1129.	12.6	4,435
2	Assembly of Metalâ€“Organic Frameworks (MOFs) Based on Indium-Trimer Building Blocks: A Porous MOF with soc Topology and High Hydrogen Storage. Angewandte Chemie - International Edition, 2007, 46, 3278-3283.	13.8	633
3	Zeolite-like Metalâ^'Organic Frameworks (ZMOFs) as Hydrogen Storage Platform: Lithium and Magnesium Ion-Exchange and H₂-(rho-ZMOF) Interaction Studies. Journal of the American Chemical Society, 2009, 131, 2864-2870.	13.7	456
4	Enhancing H₂ Uptake by â€œCloseâ€Packingâ€•Alignment of Open Copper Sites in Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2008, 47, 7263-7266.	13.8	306
5	Characterization of H2Binding Sites in Prototypical Metalâ^'Organic Frameworks by Inelastic Neutron Scattering. Journal of the American Chemical Society, 2005, 127, 14904-14910.	13.7	285
6	Hydrogen Storage in New Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2012, 116, 13143-13151.	3.1	174
7	Interaction of hydrogen with accessible metal sites in the metalâ€“organic frameworks M2(dhtp) (CPO-27-M; M = Ni, Co, Mg). Chemical Communications, 2010, 46, 4962.	4.1	173
8	Further Investigation of the Effect of Framework Catenation on Hydrogen Uptake in Metalâ^'Organic Frameworks. Journal of the American Chemical Society, 2008, 130, 15896-15902.	13.7	148
9	On Demand: The Singular rht Net, an Ideal Blueprint for the Construction of a Metalâ€“Organic Framework (MOF) Platform. Angewandte Chemie - International Edition, 2012, 51, 10099-10103.	13.8	116
10	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
11	Barrier to rotation of the dihydrogen ligand in metal complexes. The Journal of Physical Chemistry, 1993, 97, 2378-2384.	2.9	77
12	Observation of Exceptionally Strong Binding of Molecular Hydrogen in a Porous Material:Â Formation of an Î·2-H2Complex in a Cu-Exchanged ZSM-5 Zeolite. Journal of the American Chemical Society, 2007, 129, 8086-8087.	13.7	69
13	Breathers or Structural Instability in Solid L-Alanine:Â a New IR and Inelastic Neutron Scattering Vibrational Spectroscopic Study. Journal of Physical Chemistry A, 2002, 106, 5230-5241.	2.5	60
14	Reversible Displacement of Polyagostic Interactions in 16e [Mn(CO)(R2PC2H4PR2)2]+by H2, N2, and SO2. Binding and Activation of Î·2-H2trans to CO Is Nearly Invariant to Changes in Charge and cis Ligands. Inorganic Chemistry, 1999, 38, 1069-1084.	4.0	55
15	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
16	Adsorption of Hydrogen in Ca-Exchanged Na-A Zeolites Probed by Inelastic Neutron Scattering Spectroscopy. The Journal of Physical Chemistry, 1996, 100, 10646-10651.	2.9	47
17	Hydrogen adsorbed in a metal organic framework-5: Coupled translation-rotation eigenstates from quantum five-dimensional calculations. Journal of Chemical Physics, 2012, 137, 014701.	3.0	43
18	A manganese hydride molecular sieve for practical hydrogen storage under ambient conditions. Energy and Environmental Science, 2019, 12, 1580-1591.	30.8	41

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19	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
20	Capturing the H₂â€“Metal Interaction in Mg-MOF-74 Using Classical Polarization. Journal of Physical Chemistry C, 2014, 118, 22683-22690.	3.1	40
21	Computational study of molecular hydrogen in zeolite Na-A. I. Potential energy surfaces and thermodynamic separation factors for ortho and para hydrogen. Journal of Chemical Physics, 1999, 111, 7599-7613.	3.0	37
22	Infrared and Inelastic Neutron Scattering Study of the 1.03- and 0.95-nm Kaoliniteâ˜'Hydrazine Intercalation Complexes. Journal of Physical Chemistry B, 2000, 104, 8080-8088.	2.6	34
23	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
24	Computational study of molecular hydrogen in zeolite Naâ€“A. II. Density of rotational states and inelastic neutron scattering spectra. Journal of Chemical Physics, 2001, 114, 10137-10150.	3.0	28
25	A high rotational barrier for physisorbed hydrogen in an fcu-metalâ€“organic framework. Chemical Communications, 2014, 50, 14109-14112.	4.1	28
26	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
27	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
28	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
29	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
30	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
31	Origin of the Enhanced Interaction of Molecular Hydrogen with Extraframework Cu⁺ and FeO⁺ Cations in Zeolite Hosts. A Periodic DFT Study. Journal of Physical Chemistry C, 2010, 114, 13926-13934.	3.1	20
32	The rotational dynamics of H₂ adsorbed in covalent organic frameworks. Physical Chemistry Chemical Physics, 2017, 19, 13075-13082.	2.8	17
33	Hydrogen Adsorption in a Zeolitic Imidazolate Framework with lta Topology. Journal of Physical Chemistry C, 2018, 122, 15435-15445.	3.1	17
34	Probing the dynamics of complexed local anesthetics via neutron scattering spectroscopy and DFT calculations. International Journal of Pharmaceutics, 2017, 524, 397-406.	5.2	14
35	Raman and Infrared spectroscopies and X-ray diffraction data on bupivacaine and ropivacaine complexed with 2-hydroxypropylâ˜'Î²â˜'cyclodextrin. Data in Brief, 2017, 15, 25-29.	1.0	14
36	High H₂ Sorption Energetics in Zeolitic Imidazolate Frameworks. Journal of Physical Chemistry C, 2017, 121, 1723-1733.	3.1	13

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37	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
38	Interaction of Hydrogen with Extraframework Cations in Zeolite Hosts Probed by Inelastic Neutron Scattering Spectroscopy. Journal of Nanoscience and Nanotechnology, 2010, 10, 49-59.	0.9	9
39	Ammonia Storage in Hydrogen Bond-Rich Microporous Polymers. ACS Applied Materials & Interfaces, 2020, 12, 58161-58169.	8.0	9
40	Restricted mobility of specific functional groups reduces anti-cancer drug activity in healthy cells. Scientific Reports, 2016, 6, 22478.	3.3	8
41	Computational study of inelastic neutron scattering vibrational spectra of water clusters and their relevance to hydration water in proteins. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 3564-3572.	2.4	7
42	Hydrogen bonds in crystalline <scp>D</scp>-alanine: diffraction and spectroscopic evidence for differences between enantiomers. IUCrJ, 2018, 5, 6-12.	2.2	7
43	Methyl Dynamics Flattens Barrier to Proton Transfer in Crystalline Tetraacetylethane. Journal of Physical Chemistry A, 2012, 116, 2283-2291.	2.5	6
44	Hydrogen Storage Materials. Neutron Scattering Applications and Techniques, 2015, , 205-239.	0.2	5
45	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
46	A quantum dynamical study of the rotation of the dihydrogen ligand in the Fe(H)2(H2)(PEtPh2)3 coordination complex. Journal of Chemical Physics, 2018, 148, 154303.	3.0	4
47	Hydrogen bond dynamics and conformational flexibility in antipsychotics. Physical Chemistry Chemical Physics, 2019, 21, 15463-15470.	2.8	4
48	Mutual interactions in a ternary protein/bioprotectant/water system. Vibrational Spectroscopy, 2018, 99, 190-195.	2.2	1
49	Response to comment on `Hydrogen bonds in crystalline D-alanine: diffraction and spectroscopic evidence for differences between enantiomers'. IUCrJ, 2018, 5, 658-659.	2.2	0