Dewi W Lewis

List of Publications by Year
in descending order

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80 papers	4,394 citations	136950 32 h-index	106344 65 g-index
88 all docs	88 docs citations	88 times ranked	4491 citing authors

#	Article	IF	Citations
1	Single-Site Heterogeneous Catalysts. Angewandte Chemie - International Edition, 2005, 44, 6456-6482.	13.8	804
2	De novo design of structure-directing agents for the synthesis of microporous solids. Nature, 1996, 382, 604-606.	27.8	302
3	Zeolitic Polyoxometalate-Based Metalâ^'Organic Frameworks (Z-POMOFs): Computational Evaluation of Hypothetical Polymorphs and the Successful Targeted Synthesis of the Redox-Active Z-POMOF1. Journal of the American Chemical Society, 2009, 131, 16078-16087.	13.7	265
4	Zeolitic imidazole frameworks: structural and energetics trends compared with their zeolite analogues. CrystEngComm, 2009, 11, 2272.	2.6	217
5	Modeling of Silicon Substitution in SAPO-5 and SAPO-34 Molecular Sieves. Journal of Physical Chemistry B, 1997, 101, 5249-5262.	2.6	179
6	Enhancing the Enantioselectivity of Novel Homogeneous Organometallic Hydrogenation Catalysts. Angewandte Chemie - International Edition, 2003, 42, 4326-4331.	13.8	177
7	Step-wise dealumination of natural clinoptilolite: Structural and physicochemical characterization. Microporous and Mesoporous Materials, 2010, 135, 187-196.	4.4	129
8	Structure and Stability of Silica Species in SAPO Molecular Sieves. The Journal of Physical Chemistry, 1996, 100, 6722-6730.	2.9	115
9	Computer Modeling of Nucleation, Growth, and Templating in Hydrothermal Synthesis. Chemistry of Materials, 1998, 10, 3249-3265.	6.7	109
10	Oligomerization and Cyclization Processes in the Nucleation of Microporous Silicas. Angewandte Chemie - International Edition, 2005, 44, 3082-3086.	13.8	106
11	Synthesis of a Small-Pore Microporous Material Using a Computationally Designed Template. Angewandte Chemie International Edition in English, 1997, 36, 2675-2677.	4.4	85
12	Solvent-Free Routes to Clean Technology. Chemistry - A European Journal, 2001, 7, 2972-2978.	3.3	85
13	Structure of Iron-Substituted ZSM-5. The Journal of Physical Chemistry, 1995, 99, 2377-2383.	2.9	79
14	Modelling of Brnsted acidity in AFI and CHA zeotypes. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 3049-3058.	1.7	74
15	Influence of Organic Templates on the Structure and on the Concentration of Framework Metal Ions in Microporous Aluminophosphate Catalysts. Chemistry of Materials, 1996, 8, 1112-1118.	6.7	72
16	Modeling Aqueous Silica Chemistry in Alkali Media. Journal of Physical Chemistry C, 2007, 111, 18155-18158.	3.1	70
17	Synchrotron-Based Method for the Study of Crystallization: Templated Formation of CoALPO-5 Catalyst. Chemistry of Materials, 1995, 7, 1435-1436.	6.7	68
18	Mechanisms of silicon incorporation in aluminophosphate molecular sieves. Journal of Molecular Catalysis A, 1997, 119, 349-356.	4.8	60

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19	Application of computer modelling to the mechanisms of synthesis of microporous catalytic materials. Faraday Discussions, 1997, 106, 451-471.	3.2	58
20	Probing the Acid Strength of BrÃ¸nsted Acidic Zeolites with Acetonitrile:Â An Atomistic and Quantum Chemical Study. Journal of Physical Chemistry B, 2004, 108, 7152-7161.	2.6	58
21	Zeolitic polyoxometalates metal organic frameworks (Z-POMOF) with imidazole ligands and Îµ-Keggin ions as building blocks; computational evaluation of hypothetical polymorphs and a synthesis approach. Physical Chemistry Chemical Physics, 2010, 12, 8632.	2.8	51
22	Zeolite-Modified Discriminating Gas Sensors. Journal of the Electrochemical Society, 2009, 156, J46.	2.9	49
23	Structure of Zeolite A (LTA) Surfaces and the Zeolite A/Water Interface. Journal of Physical Chemistry C, 2010, 114, 9739-9747.	3.1	43
24	Aluminum Distribution in Low Si/Al Zeolites:â€‰ Dehydrated Naâ^'Clinoptilolite. Journal of Physical Chemistry B, 1998, 102, 8417-8425.	2.6	41
25	Classical simulations of the properties of group-III nitrides. Journal of Physics Condensed Matter, 1999, 11, L235-L239.	1.8	39
26	Modelling of structure and reactivity in zeolites. Studies in Surface Science and Catalysis, 1995, 97, 87-100.	1.5	38
27	Designing templates for the synthesis of microporous solids using de novo molecular design methods. Journal of Molecular Catalysis A, 1997, 119, 415-424.	4.8	38
28	On the nature of iron species in iron substituted aluminophosphates. Physical Chemistry Chemical Physics, 2002, 4, 5421-5429.	2.8	36
29	Probing ZnAPO-34 Self-Assembly Using Simultaneous Multiple in Situ Techniques. Journal of Physical Chemistry C, 2011, 115, 6331-6340.	3.1	35
30	Benign by design. New catalysts for an environmentally conscious age. Pure and Applied Chemistry, 2001, 73, 1087-1101.	1.9	34
31	Discrimination Effects in Zeolite Modified Metal Oxide Semiconductor Gas Sensors. IEEE Sensors Journal, 2011, 11, 1145-1151.	4.7	34
32	Space group symmetry and Alâ€"Oâ€"P bond angles in AlPO4-5. Journal of Materials Chemistry, 1996, 6, 1837-1842.	6.7	31
33	The Adsorption of CO on the Stepped Pt{211} Surface: A Comparison of Theory and Experiment. Catalysis Letters, 2003, 88, 39-45.	2.6	30
34	Clinoptiloliteâ€"heulandite polymorphism: structural features from computer simulation. Physical Chemistry Chemical Physics, 2000, 2, 1803-1813.	2.8	28
35	Synthesis, characterisation and catalytic performance of the solid acid DAF-1. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 3537.	1.7	27
36	Pressure-Induced Hydration Effects in the Zeolite Laumontite. Angewandte Chemie - International Edition, 2004, 43, 469-472.	13.8	26

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37	Modelling of hydrated Ca-rich zeolites. Molecular Simulation, 2002, 28, 649-661.	2.0	24
38	Effect of Organic Templates on the Kinetics and Crystallization of Microporous Metal-Substituted Aluminophosphates. Journal of Physical Chemistry C, 2007, 111, 16951-16961.	3.1	24
39	Spiral Growth on Nanoporous Silicoaluminophosphate STA-7 as Observed by Atomic Force Microscopy. Crystal Growth and Design, 2009, 9, 4041-4050.	3.0	24
40	Surprising role of the BDC organic ligand in the adsorption of CO2 by MOF-5. Microporous and Mesoporous Materials, 2012, 163, 186-191.	4.4	24
41	Understanding Si/Al distributions in Al-rich zeolites: the role of water in determining the structure of Goosecreekite. Chemical Communications, 2001, , 531-532.	4.1	23
42	Siliconâ€“aluminium distribution in dehydrated calcium heulandite. Physical Chemistry Chemical Physics, 1999, 1, 1679-1685.	2.8	22
43	Interplay of water, extra-framework cations and framework atoms in the structure of low-silicazeolites: the case of the natural zeolite Goosecreekite as studied by computer simulation. Physical Chemistry Chemical Physics, 2007, 9, 521-532.	2.8	21
44	Modifying the Crystal Habit of Zeolite L by Addition of an Organic Space Filler. Journal of Physical Chemistry C, 2010, 114, 18240-18246.	3.1	21
45	Aluminium distribution in ZSM-5 revisited: The role of Alâ€“Al interactions. Journal of Solid State Chemistry, 2013, 198, 330-336.	2.9	21
46	Structure of templated microcrystalline DAF-5â€ (Co0.28Al0.72PO4C10H20N2) determined by synchrotron-based diffraction methods. Chemical Communications, 1998, , 117-118.	4.1	20
47	Rationalisation of the IR stretching frequencies of BrÃ¸nsted acid centres in microporous solids. Chemical Communications, 1999, , 349-350.	4.1	20
48	Probing the Structural and Binding Mechanism Heterogeneity of Molecularly Imprinted Polymers. Journal of Physical Chemistry B, 2015, 119, 563-571.	2.6	20
49	The role of the electrostatic potential, electric field and electric field gradient on the acidity of AFI and CHA zeotypes. Physical Chemistry Chemical Physics, 2000, 2, 177-185.	2.8	18
50	H-Bond interactions between silicates and water during zeolite pre-nucleation. Physical Chemistry Chemical Physics, 2008, 10, 6571.	2.8	17
51	Computer simulation of Fe-ZSM5 â€" comparison to EXAFS studies. Nuclear Instruments & Methods in Physics Research B, 1995, 97, 44-49.	1.4	16
52	Role of Germanium on the Nucleation and Growth of Zeolite A from Clear Solutions As Studied by in Situ Small-Angle X-ray Scattering, Wide-Angle X-ray Scattering, and Dynamic Light Scattering. Journal of Physical Chemistry C, 2009, 113, 18614-18622.	3.1	16
53	Modelling of structure, sorption, synthesis and reactivity in catalytic systems1Communication presented at the First Francqui Colloquium, Brussels, 19â€"20 February 1996.1. Journal of Molecular Catalysis A, 1997, 115, 431-448.	4.8	13
54	Towards Rational Design of Solid Acid Catalysts. Zeitschrift Fur Physikalische Chemie, 1996, 197, 37-48.	2.8	12

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55	The role of organic templates in controlling zeolite crystal morphology. Studies in Surface Science and Catalysis, 2007, , 1685-1692.	1.5	12
56	Pressure-induced structural transformations of the Zintl phase sodium silicide. Journal of Solid State Chemistry, 2009, 182, 2535-2542.	2.9	12
57	Defect processes at low coordinate surface sites of MgO and their role in the partial oxidation of hydrocarbons. Journal of Molecular Catalysis A, 1995, 100, 103-114.	4.8	11
58	Synthese eines kleinporigen mikroporÃ¶sen Materials unter Verwendung eines computerâ€gestÃ¼tzt entworfenen Templats. Angewandte Chemie, 1997, 109, 2791-2793.	2.0	11
59	Gas Sensing Properties of Composite Tungsten Trioxide-Zeolite Thick Films. ECS Transactions, 2009, 16, 77-84.	0.5	10
60	A computational study of the role of chlorine in the partial oxidation of methane by MgO and Li/MgO. Topics in Catalysis, 1994, 1, 111-121.	2.8	9
61	Calculation of the ²⁹Si NMR Chemical Shifts of Aqueous Silicate Species. Journal of Physical Chemistry A, 2012, 116, 8786-8791.	2.5	8
62	Simultaneous occupation of SI and SIâ€² cation sites in dehydrated zeolite LSX. Chemical Communications, 2002, , 2660-2661.	4.1	7
63	Zeolites as transformation elements in discriminating semiconductor metal oxide sensors. Procedia Engineering, 2010, 5, 103-106.	1.2	7
64	Computer modelling of the structure and synthesis of microporous and mesoporous materials. Studies in Surface Science and Catalysis, 1997, 105, 2291-2298.	1.5	5
65	Design of microporous transition metal oxide catalysts and investigation of their synthesis conditions. Journal of Molecular Catalysis A, 2001, 166, 123-134.	4.8	5
66	Si atoms in SAPO-31: A computational study. Studies in Surface Science and Catalysis, 2004, 154, 1439-1447.	1.5	5
67	Zeolite-based discriminating gas sensors. Studies in Surface Science and Catalysis, 2008, 174, 549-554.	1.5	4
68	Probing the structure of complex solids using a distributed computing approachâ€”Applications in zeolite science. Journal of Solid State Chemistry, 2011, 184, 1484-1491.	2.9	4
69	De novo design of microporous transition metal oxides. Chemical Communications, 1998, , 1943-1944.	4.1	3
70	Approaching the structure of heavily defective ionic oxides through atomistic modeling. Physica Status Solidi C: Current Topics in Solid State Physics, 2005, 2, 3521-3524.	0.8	3
71	Location and orientation of the N,N-diisopropylethylamine template molecule in the AlPO4-18 framework by X-ray synchrotron diffraction and molecular modelling. Chinese Journal of Catalysis, 2015, 36, 874-879.	14.0	3
72	Screening heteroatom distributions in zeotype materials using an effective Hamiltonian approach: the case of aluminogermanate PKU-9. Physical Chemistry Chemical Physics, 2018, 20, 18047-18055.	2.8	3

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73	Effect of hydration levels and pressure on zeolite structure. Studies in Surface Science and Catalysis, 2004, 154, 1737-1745.	1.5	2
74	29Si NMR chemical shifts from Density Functional Theory incorporating solvent effects. Studies in Surface Science and Catalysis, 2008, , 725-728.	1.5	2
75	Chemical insertion in the perovskite solid solutions Pr0.5+xâ^'yLi0.5â^'3xBiyâ–¡2xTiO3: Implications on the electrical properties. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2012, 177, 563-569.	3.5	2
76	Template-host interaction and template design. , 2004, , 243-265.		1
77	Single-Site Heterogeneous Catalysts. ChemInform, 2006, 37, no.	0.0	1
78	Discrimination effects in zeolite modified metal oxide semiconductor gas sensors. , 2009, , .		1
79	Modeling Nucleation and Growth in Zeolites. , 2003, , .		1
80	Influence of cations on crystal growth mechanism: ABW vs. JBW. Studies in Surface Science and Catalysis, 2007, 170, 674-681.	1.5	0