

Dewi W Lewis

List of Publications by Year in descending order

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80
papers

4,394
citations

136950

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106344

65
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88
all docs

88
docs citations

88
times ranked

4491
citing authors

#	ARTICLE	IF	CITATIONS
1	Screening heteroatom distributions in zeotype materials using an effective Hamiltonian approach: the case of aluminogermanate PKU-9. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 18047-18055.	2.8	3
2	Location and orientation of the N,N-diisopropylethylamine template molecule in the AlPO4-18 framework by X-ray synchrotron diffraction and molecular modelling. <i>Chinese Journal of Catalysis</i> , 2015, 36, 874-879.	14.0	3
3	Probing the Structural and Binding Mechanism Heterogeneity of Molecularly Imprinted Polymers. <i>Journal of Physical Chemistry B</i> , 2015, 119, 563-571.	2.6	20
4	Aluminium distribution in ZSM-5 revisited: The role of Al-Al interactions. <i>Journal of Solid State Chemistry</i> , 2013, 198, 330-336.	2.9	21
5	Surprising role of the BDC organic ligand in the adsorption of CO2 by MOF-5. <i>Microporous and Mesoporous Materials</i> , 2012, 163, 186-191.	4.4	24
6	Calculation of the ²⁹ Si NMR Chemical Shifts of Aqueous Silicate Species. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8786-8791.	2.5	8
7	Chemical insertion in the perovskite solid solutions Pr _{0.5+x} Li _{0.5-3x} Biy- ₂ TiO ₃ : Implications on the electrical properties. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2012, 177, 563-569.	3.5	2
8	Discrimination Effects in Zeolite Modified Metal Oxide Semiconductor Gas Sensors. <i>IEEE Sensors Journal</i> , 2011, 11, 1145-1151.	4.7	34
9	Probing ZnAPO-34 Self-Assembly Using Simultaneous Multiple in Situ Techniques. <i>Journal of Physical Chemistry C</i> , 2011, 115, 6331-6340.	3.1	35
10	Probing the structure of complex solids using a distributed computing approach Applications in zeolite science. <i>Journal of Solid State Chemistry</i> , 2011, 184, 1484-1491.	2.9	4
11	Zeolites as transformation elements in discriminating semiconductor metal oxide sensors. <i>Procedia Engineering</i> , 2010, 5, 103-106.	1.2	7
12	Step-wise dealumination of natural clinoptilolite: Structural and physicochemical characterization. <i>Microporous and Mesoporous Materials</i> , 2010, 135, 187-196.	4.4	129
13	Structure of Zeolite A (LTA) Surfaces and the Zeolite A/Water Interface. <i>Journal of Physical Chemistry C</i> , 2010, 114, 9739-9747.	3.1	43
14	Zeolitic polyoxometalates metal organic frameworks (Z-POMOF) with imidazole ligands and μ -Keggin ions as building blocks; computational evaluation of hypothetical polymorphs and a synthesis approach. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 8632.	2.8	51
15	Modifying the Crystal Habit of Zeolite L by Addition of an Organic Space Filler. <i>Journal of Physical Chemistry C</i> , 2010, 114, 18240-18246.	3.1	21
16	Discrimination effects in zeolite modified metal oxide semiconductor gas sensors. , 2009, , .		1
17	Pressure-induced structural transformations of the Zintl phase sodium silicide. <i>Journal of Solid State Chemistry</i> , 2009, 182, 2535-2542.	2.9	12
18	Spiral Growth on Nanoporous Silicoaluminophosphate STA-7 as Observed by Atomic Force Microscopy. <i>Crystal Growth and Design</i> , 2009, 9, 4041-4050.	3.0	24

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19	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. <i>Journal of Physical Chemistry C</i> , 2009, 113, 18614-18622.	3.1	16
20	Zeolitic imidazole frameworks: structural and energetics trends compared with their zeolite analogues. <i>CrystEngComm</i> , 2009, 11, 2272.	2.6	217
21	Zeolitic Polyoxometalate-Based Metal-Organic Frameworks (Z-POMOFs): Computational Evaluation of Hypothetical Polymorphs and the Successful Targeted Synthesis of the Redox-Active Z-POMOF1. <i>Journal of the American Chemical Society</i> , 2009, 131, 16078-16087.	13.7	265
22	Gas Sensing Properties of Composite Tungsten Trioxide-Zeolite Thick Films. <i>ECS Transactions</i> , 2009, 16, 77-84.	0.5	10
23	Zeolite-Modified Discriminating Gas Sensors. <i>Journal of the Electrochemical Society</i> , 2009, 156, J46.	2.9	49
24	Zeolite-based discriminating gas sensors. <i>Studies in Surface Science and Catalysis</i> , 2008, 174, 549-554.	1.5	4
25	H-Bond interactions between silicates and water during zeolite pre-nucleation. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 6571.	2.8	17
26	²⁹ Si NMR chemical shifts from Density Functional Theory incorporating solvent effects. <i>Studies in Surface Science and Catalysis</i> , 2008, , 725-728.	1.5	2
27	The role of organic templates in controlling zeolite crystal morphology. <i>Studies in Surface Science and Catalysis</i> , 2007, , 1685-1692.	1.5	12
28	Influence of cations on crystal growth mechanism: ABW vs. JBW. <i>Studies in Surface Science and Catalysis</i> , 2007, 170, 674-681.	1.5	0
29	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. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 521-532.	2.8	21
30	Effect of Organic Templates on the Kinetics and Crystallization of Microporous Metal-Substituted Aluminophosphates. <i>Journal of Physical Chemistry C</i> , 2007, 111, 16951-16961.	3.1	24
31	Modeling Aqueous Silica Chemistry in Alkali Media. <i>Journal of Physical Chemistry C</i> , 2007, 111, 18155-18158.	3.1	70
32	Single-Site Heterogeneous Catalysts. <i>ChemInform</i> , 2006, 37, no.	0.0	1
33	Single-Site Heterogeneous Catalysts. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 6456-6482.	13.8	804
34	Oligomerization and Cyclization Processes in the Nucleation of Microporous Silicas. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 3082-3086.	13.8	106
35	Approaching the structure of heavily defective ionic oxides through atomistic modeling. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2005, 2, 3521-3524.	0.8	3
36	Si atoms in SAPO-31: A computational study. <i>Studies in Surface Science and Catalysis</i> , 2004, 154, 1439-1447.	1.5	5

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37	Pressure-Induced Hydration Effects in the Zeolite Laumontite. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 469-472.	13.8	26
38	Effect of hydration levels and pressure on zeolite structure. <i>Studies in Surface Science and Catalysis</i> , 2004, 154, 1737-1745.	1.5	2
39	Probing the Acid Strength of Brønsted Acidic Zeolites with Acetonitrile: An Atomistic and Quantum Chemical Study. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7152-7161.	2.6	58
40	Template-host interaction and template design. , 2004, , 243-265.		1
41	The Adsorption of CO on the Stepped Pt{211} Surface: A Comparison of Theory and Experiment. <i>Catalysis Letters</i> , 2003, 88, 39-45.	2.6	30
42	Enhancing the Enantioselectivity of Novel Homogeneous Organometallic Hydrogenation Catalysts. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 4326-4331.	13.8	177
43	Modeling Nucleation and Growth in Zeolites. , 2003, , .		1
44	Modelling of hydrated Ca-rich zeolites. <i>Molecular Simulation</i> , 2002, 28, 649-661.	2.0	24
45	On the nature of iron species in iron substituted aluminophosphates. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5421-5429.	2.8	36
46	Simultaneous occupation of SI and Si ²⁺ cation sites in dehydrated zeolite LSX. <i>Chemical Communications</i> , 2002, , 2660-2661.	4.1	7
47	Understanding Si/Al distributions in Al-rich zeolites: the role of water in determining the structure of Goosecreekite. <i>Chemical Communications</i> , 2001, , 531-532.	4.1	23
48	Benign by design. New catalysts for an environmentally conscious age. <i>Pure and Applied Chemistry</i> , 2001, 73, 1087-1101.	1.9	34
49	Design of microporous transition metal oxide catalysts and investigation of their synthesis conditions. <i>Journal of Molecular Catalysis A</i> , 2001, 166, 123-134.	4.8	5
50	Solvent-Free Routes to Clean Technology. <i>Chemistry - A European Journal</i> , 2001, 7, 2972-2978.	3.3	85
51	Clinoptilolite ⁺ heulandite polymorphism: structural features from computer simulation. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 1803-1813.	2.8	28
52	The role of the electrostatic potential, electric field and electric field gradient on the acidity of AFI and CHA zeotypes. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 177-185.	2.8	18
53	Classical simulations of the properties of group-III nitrides. <i>Journal of Physics Condensed Matter</i> , 1999, 11, L235-L239.	1.8	39
54	Silicon ⁺ aluminium distribution in dehydrated calcium heulandite. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 1679-1685.	2.8	22

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55	Rationalisation of the IR stretching frequencies of Brønsted acid centres in microporous solids. <i>Chemical Communications</i> , 1999, , 349-350.	4.1	20
56	De novo design of microporous transition metal oxides. <i>Chemical Communications</i> , 1998, , 1943-1944.	4.1	3
57	Structure of templated microcrystalline DAF-5 (Co _{0.28} Al _{0.72} PO ₄ C ₁₀ H ₂₀ N ₂) determined by synchrotron-based diffraction methods. <i>Chemical Communications</i> , 1998, , 117-118.	4.1	20
58	Modelling of Brønsted acidity in AFI and CHA zeotypes. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1998, 94, 3049-3058.	1.7	74
59	Computer Modeling of Nucleation, Growth, and Templating in Hydrothermal Synthesis. <i>Chemistry of Materials</i> , 1998, 10, 3249-3265.	6.7	109
60	Aluminum Distribution in Low Si/Al Zeolites: Dehydrated Na ⁺ Clinoptilolite. <i>Journal of Physical Chemistry B</i> , 1998, 102, 8417-8425.	2.6	41
61	Computer modelling of the structure and synthesis of microporous and mesoporous materials. <i>Studies in Surface Science and Catalysis</i> , 1997, 105, 2291-2298.	1.5	5
62	Application of computer modelling to the mechanisms of synthesis of microporous catalytic materials. <i>Faraday Discussions</i> , 1997, 106, 451-471.	3.2	58
63	Modeling of Silicon Substitution in SAPO-5 and SAPO-34 Molecular Sieves. <i>Journal of Physical Chemistry B</i> , 1997, 101, 5249-5262.	2.6	179
64	Modelling of structure, sorption, synthesis and reactivity in catalytic systems1Communication presented at the First Francqui Colloquium, Brussels, 19 th February 1996.1. <i>Journal of Molecular Catalysis A</i> , 1997, 115, 431-448.	4.8	13
65	Mechanisms of silicon incorporation in aluminophosphate molecular sieves. <i>Journal of Molecular Catalysis A</i> , 1997, 119, 349-356.	4.8	60
66	Designing templates for the synthesis of microporous solids using de novo molecular design methods. <i>Journal of Molecular Catalysis A</i> , 1997, 119, 415-424.	4.8	38
67	Synthesis of a Small-Pore Microporous Material Using a Computationally Designed Template. <i>Angewandte Chemie International Edition in English</i> , 1997, 36, 2675-2677.	4.4	85
68	Synthese eines kleinporigen mikroporösen Materials unter Verwendung eines computerergestützten entworfenen Templats. <i>Angewandte Chemie</i> , 1997, 109, 2791-2793.	2.0	11
69	Structure and Stability of Silica Species in SAPO Molecular Sieves. <i>The Journal of Physical Chemistry</i> , 1996, 100, 6722-6730.	2.9	115
70	Influence of Organic Templates on the Structure and on the Concentration of Framework Metal Ions in Microporous Aluminophosphate Catalysts. <i>Chemistry of Materials</i> , 1996, 8, 1112-1118.	6.7	72
71	Space group symmetry and Al-O-P bond angles in AlPO ₄ -5. <i>Journal of Materials Chemistry</i> , 1996, 6, 1837-1842.	6.7	31
72	De novo design of structure-directing agents for the synthesis of microporous solids. <i>Nature</i> , 1996, 382, 604-606.	27.8	302

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73	Towards Rational Design of Solid Acid Catalysts. Zeitschrift Fur Physikalische Chemie, 1996, 197, 37-48.	2.8	12
74	Modelling of structure and reactivity in zeolites. Studies in Surface Science and Catalysis, 1995, 97, 87-100.	1.5	38
75	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
76	Computer simulation of Fe-ZSM5 " comparison to EXAFS studies. Nuclear Instruments & Methods in Physics Research B, 1995, 97, 44-49.	1.4	16
77	Structure of Iron-Substituted ZSM-5. The Journal of Physical Chemistry, 1995, 99, 2377-2383.	2.9	79
78	Synchrotron-Based Method for the Study of Crystallization: Templated Formation of CoALPO-5 Catalyst. Chemistry of Materials, 1995, 7, 1435-1436.	6.7	68
79	Synthesis, characterisation and catalytic performance of the solid acid DAF-1. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 3537.	1.7	27
80	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