German Sastre

List of Publications by Year in Descending Order

154 papers	4,420 citations	41 h-index	58 g-index
162 ext. papers	4,855 ext. citations	5.8 avg, IF	5.65 L-index

#	Paper	IF	Citations
154	Zeolite Phase Selectivity Using the Same Organic Structure-Directing Agent in Fluoride and Hydroxide Media. *Journal of Physical Chemistry C*, **2022**, 126, 2078-2087	3.8	1
153	Stereoselective, Ruthenium-Photocatalyzed Synthesis of 1,2-Diaminotruxinic Bis-amino Acids from 4-Arylidene-5(4)-oxazolones.. *Journal of Organic Chemistry*, **2022**,	4.2	3
152	Synergistically enhance confined diffusion by continuum intersecting channels in zeolites. *Science Advances*, **2021**, 7,	14.3	11
151	Connecting theory and simulation with experiment for the study of diffusion in nanoporous solids. *Adsorption*, **2021**, 27, 683-760	2.6	25
150	Separation of an aqueous mixture of 6-kestose/sucrose with zeolites: A molecular dynamics simulation. *Microporous and Mesoporous Materials*, **2021**, 319, 111031	5.3	2
149	Thermal resistance effect on anomalous diffusion of molecules under confinement. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	4
148	Surface barriers and symmetry of adsorption and desorption processes. *Adsorption*, **2021**, 27, 777-785	2.6	9
147	Computational elucidation of the aging time effect on zeolite synthesis selectivity in the presence of water and diquaternary ammonium iodide. *Physical Chemistry Chemical Physics*, **2021**, 23, 21240-21248	3.6	
146	Control of zeolite microenvironment for propene synthesis from methanol. *Nature Communications*, **2021**, 12, 822	17.4	5
145	Diffusivity of Propylene in One-Dimensional Medium-Pore Zeolites. *Journal of Physical Chemistry C*, **2021**, 125, 19200-19208	3.8	0
144	Identification of New Templates for the Synthesis of BEA, BEC, and ISV Zeolites Using Molecular Topology and Monte Carlo Techniques. *Journal of Chemical Information and Modeling*, **2020**, 60, 2819-2829	6.1	2
143	Light Olefin Diffusion during the MTO Process on H-SAPO-34: A Complex Interplay of Molecular Factors. *Journal of the American Chemical Society*, **2020**, 142, 6007-6017	16.4	48
142	Evidence of Hydronium Formation in Water Chabazite Zeolite Using Inelastic Neutron Scattering Experiments and ab Initio Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2020**, 124, 5436-5443	3.8	5
141	Sequential pore wall functionalization in covalent organic frameworks and application to stable camptothecin delivery systems. *Materials Science and Engineering C*, **2020**, 117, 111263	8.3	4
140	Computational Screening of Structure-Directing Agents for the Synthesis of Pure Silica ITE Zeolite. *Journal of Physical Chemistry Letters*, **2020**, 11, 6164-6167	6.4	1
139	Insights into Adsorption of Linear, Monobranched, and Dibranched Alkanes on Pure Silica STW Zeolite as a Promising Material for Their Separation. *Journal of Physical Chemistry C*, **2020**, 124, 26821-26829	3.8	5
138	Look beneath the surface. *Nature Materials*, **2020**, 19, 1040-1041	27	3

137	Inelastic Neutron Scattering Study of Br□sted Acidity and Water Confinement in Zeolites. *Proceedings (mdpi)*, **2019**, 26, 47	0.3	
136	Dynamic Studies on Kinetic H /D Quantum Sieving in a Narrow Pore Metal-Organic Framework Grown on a Sensor Chip. *Chemistry - A European Journal*, **2019**, 25, 10803-10807	4.8	6
135	Generation of the Thymine Triplet State by Through-Bond Energy Transfer. *Chemistry - A European Journal*, **2019**, 25, 7004-7011	4.8	3
134	Diffusion Path Reversibility Confirms Symmetry of Surface Barriers. *Journal of Physical Chemistry C*, **2019**, 123, 19596-19601	3.8	8
133	Synthesis of High-Silica Erionite Driven by Computational Screening of Hypothetical Zeolites. *Chemistry of Materials*, **2019**, 31, 9268-9276	9.6	6
132	Computational screening of structure directing agents for the synthesis of zeolites. A simplified model. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2019**, 234, 451-460	1	9
131	Engineered contrast agents in a single structure for T-T dual magnetic resonance imaging. *Nanoscale*, **2018**, 10, 6349-6360	7.7	9
130	Molecular Dynamics Study of Diffusion and Surface Permeation of Benzene in Silicalite. *Journal of Physical Chemistry C*, **2018**, 122, 7217-7225	3.8	23
129	Molecular Dynamics of Hydrocarbons in Zeolites: Historical Perspective and Current Developments **2018**, 27-62		3
128	Zeolite structure determination using genetic algorithms and geometry optimisation. *Faraday Discussions*, **2018**, 211, 103-115	3.6	4
127	Inelastic Neutron Scattering Study of the Aluminum and Br□sted Site Location in Aluminosilicate LTA Zeolites. *Journal of Physical Chemistry C*, **2018**, 122, 11450-11454	3.8	7
126	Diffusion of Trimethylbenzenes, Toluene, and Xylenes in UWY Zeolite as a Catalyst for Transalkylation of Trimethylbenzenes with Toluene. *Journal of Physical Chemistry C*, **2018**, 122, 7885-7897	3.8	8
125	Achieving Large Volumetric Gas Storage Capacity in Metal-Organic Frameworks by Kinetic Trapping: A Case Study of Xenon Loading in MFU-4. *Journal of the American Chemical Society*, **2018**, 140, 10191-10197	16.4	35
124	Applying Genetic Algorithms in Chemical Engineering for Determining Zeolite Structures. *Advances in Intelligent Systems and Computing*, **2018**, 34-43	0.4	1
123	Applications of crystal structure prediction - inorganic and network structures: general discussion. *Faraday Discussions*, **2018**, 211, 613-642	3.6	4
122	Structure searching methods: general discussion. *Faraday Discussions*, **2018**, 211, 133-180	3.6	3
121	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. *Faraday Discussions*, **2018**, 211, 325-381	3.6	6
120	Gas confinement in compartmentalized coordination polymers for highly selective sorption. *Chemical Science*, **2017**, 8, 3109-3120	9.4	11

119	Selecting strong Brønsted acid zeolites through screening from a database of hypothetical frameworks. *Physical Chemistry Chemical Physics*, **2017**, 19, 14702-14707	3.6	6
118	Isotopic H/D exchange on graphenes. A combined experimental and theoretical study. *Applied Catalysis A: General*, **2017**, 547, 52-59	5.1	9
117	Determining zeolite structures with a domain-dependent genetic algorithm **2017**,		1
116	Calculation of pore diameters in zeolites. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	15
115	An INS study of entrapped organic cations within the micropores of zeolite RTH. *Physical Chemistry Chemical Physics*, **2016**, 18, 17244-52	3.6	4
114	Diffusion of Trimethylbenzenes and Xylenes in Zeolites with 12- and 10-Ring Channels as Catalyst for Toluene-Trimethylbenzene Transalkylation. *Journal of Physical Chemistry C*, **2016**, 120, 16668-16680	3.8	17
113	Inelastic Neutron Scattering Study on the Location of Brønsted Acid Sites in High Silica LTA Zeolite. *Journal of Physical Chemistry C*, **2016**, 120, 24904-24909	3.8	16
112	Triplet energy management between two signaling units through cooperative rigid scaffolds. *Chemical Communications*, **2016**, 52, 713-6	5.8	2
111	ITQ-39 zeolite, an efficient catalyst for the conversion of low value naphtha fractions into diesel fuel: The role of pore size on molecular diffusion and reactivity. *Journal of Catalysis*, **2016**, 333, 127-138	7.3	7
110	Confinement effects in methanol to olefins catalysed by zeolites: A computational review. *Frontiers of Chemical Science and Engineering*, **2016**, 10, 76-89	4.5	17
109	Vibrational fingerprint of the absorption properties of UiO-type MOF materials. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	7
108	Influence of force fields on the selective diffusion of para-xylene over ortho-xylene in 10-ring zeolites. *Molecular Simulation*, **2015**, 41, 1438-1448	2	13
107	Shape-Selective Diffusion of Olefins in 8-Ring Solid Acid Microporous Zeolites. *Journal of Physical Chemistry C*, **2015**, 119, 23721-23734	3.8	54
106	Configuration-Dependent Photoinduced Electron Transfer in Diastereomeric Naphthalene-Amino-Naphthalene Triads. *Chemistry - A European Journal*, **2015**, 21, 12940-6	4.8	2
105	The importance of T?T?T angles in the feasibility of zeolites. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2015**, 230, 291-299	1	21
104	Drug–tubulin interactions interrogated by transient absorption spectroscopy. *RSC Advances*, **2015**, 5, 49451-49458	3.7	2
103	Steric shielding of orbital interactions in triplet-triplet energy transfer. *Chemical Science*, **2015**, 6, 4035-4041	9.1	6
102	Computational study of diffusion of propane in small pore acidic zeotypes AFX and AEI. *Catalysis Today*, **2014**, 226, 25-36	5.3	16

101	Dielectric Relaxation Processes, Electronic Structure, and Band Gap Engineering of MFU-4-type Metal-Organic Frameworks: Towards a Rational Design of Semiconducting Microporous Materials. *Advanced Functional Materials*, **2014**, 24, 3885-3896	15.6	86
100	Screening of hypothetical metal-organic frameworks for H2 storage. *Physical Chemistry Chemical Physics*, **2014**, 16, 19001-10	3.6	27
99	Supra-molecular assembly of aromatic proton sponges to direct the crystallization of extra-large-pore zeotypes. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, **2014**, 470, 20140107	2.4	5
98	Unveiling the mechanism of selective gate-driven diffusion of CO2 over N2 in MFU-4 metal-organic framework. *Dalton Transactions*, **2014**, 43, 9612-9	4.3	19
97	CFA-1: the first chiral metal-organic framework containing Kuratowski-type secondary building units. *Dalton Transactions*, **2013**, 42, 10786-97	4.3	41
96	Simulating the properties of small pore silica zeolites using interatomic potentials. *Chemical Society Reviews*, **2013**, 42, 114-27	58.5	44
95	Drug-Drug Interactions within Protein Cavities Probed by Triplet-Triplet Energy Transfer. *Journal of Physical Chemistry Letters*, **2013**, 4, 1603-7	6.4	6
94	Dependence of cracking activity on the Brønsted acidity of Y zeolite: DFT study and experimental confirmation. *Catalysis Science and Technology*, **2013**, 3, 1919	5.5	29
93	Synthesis of a novel zeolite through a pressure-induced reconstructive phase transition process. *Angewandte Chemie - International Edition*, **2013**, 52, 10458-62	16.4	36
92	Water–Hydrophobic Zeolite Systems. *Journal of Physical Chemistry C*, **2012**, 116, 24916-24929	3.8	24
91	Confinement effects in the hydrogen adsorption on paddle wheel containing metal-organic frameworks. *Physical Chemistry Chemical Physics*, **2012**, 14, 2508-17	3.6	23
90	Photophysical properties of Kuratowski-type coordination compounds [M(II)Zn4Cl4(Me2bta)6] (M(II) = Zn or Ru) featuring long-lived excited electronic states. *Dalton Transactions*, **2011**, 40, 5926-38	4.3	24
89	Molecular Dynamics Simulations of the Diffusion of Small Chain Hydrocarbons in 8-Ring Zeolites. *Journal of Physical Chemistry C*, **2011**, 115, 875-884	3.8	28
88	Dansyl labeling to modulate the relative affinity of bile acids for the binding sites of human serum albumin. *Journal of Physical Chemistry B*, **2011**, 115, 10518-24	3.4	19
87	Ammonia IRMS-TPD measurements on Brønsted acidity of proton-formed SAPO-34. *Physical Chemistry Chemical Physics*, **2011**, 13, 3311-8	3.6	28
86	Atomistic Simulation of Water Intrusion–Extrusion in ITQ-4 (IFR) and ZSM-22 (TON): The Role of Silanol Defects. *Journal of Physical Chemistry C*, **2011**, 115, 21942-21953	3.8	22
85	Influence of Zeolite Surface in the Sorption of Methane from Molecular Dynamics. *Journal of Physical Chemistry C*, **2011**, 115, 13751-13758	3.8	43
84	From microscopic insights of H2 adsorption to uptake estimations in MOFs. *Physical Chemistry Chemical Physics*, **2011**, 13, 16558-68	3.6	19

83	Multifunctional hybrid organic-inorganic catalytic materials with a hierarchical system of well-defined micro- and mesopores. *Journal of the American Chemical Society*, **2010**, 132, 15011-21	16.4	163
82	Computational Study of Brønsted Acidity of Mordenite. Effect of the Electric Field on the Infrared OH Stretching Frequencies. *Journal of Physical Chemistry C*, **2010**, 114, 15424-15431	3.8	16
81	Predicting Structural Feasibility of Silica and Germania Zeolites. *Journal of Physical Chemistry C*, **2010**, 114, 1667-1673	3.8	42
80	The Structural Directing Role of Water and Hydroxyl Groups in the Synthesis of Beta Zeolite Polymorphs. *Journal of Physical Chemistry C*, **2010**, 114, 345-356	3.8	19
79	Feasibility of Pure Silica Zeolites. *Journal of Physical Chemistry C*, **2010**, 114, 19157-19168	3.8	34
78	Modular organic structure-directing agents for the synthesis of zeolites. *Science*, **2010**, 330, 1219-22	33.3	110
77	Hydrogen physisorption in metal–organic frameworks: concepts and quantum chemical calculations. *Theoretical Chemistry Accounts*, **2010**, 127, 259-270	1.9	13
76	Atomistic simulations of water and organic templates occluded during the synthesis of zeolites. *Microporous and Mesoporous Materials*, **2010**, 129, 42-53	5.3	18
75	The benefit of multipore zeolites: Catalytic behaviour of zeolites with intersecting channels of different sizes for alkylation reactions. *Journal of Catalysis*, **2009**, 268, 9-17	7.3	52
74	The confinement effect in zeolites. *Journal of Molecular Catalysis A*, **2009**, 305, 3-7		123
73	Topological Descriptor for Oxygens in Zeolites. Analysis of Ring Counting in Tetracoordinated Nets. *Journal of Physical Chemistry C*, **2009**, 113, 6398-6405	3.8	12
72	Periodic Density Functional Calculation on the Brønsted Acidity of Modified Y-Type Zeolite. *Journal of Physical Chemistry C*, **2009**, 113, 5672-5680	3.8	34
71	Atomistic Simulations of Structural Defects and Water Occluded in SSZ-74 Zeolite. *Journal of Physical Chemistry C*, **2009**, 113, 10877-10886	3.8	31
70	Correlation between Brønsted Acid Strength and Local Structure in Zeolites. *Journal of Physical Chemistry C*, **2009**, 113, 19208-19217	3.8	98
69	Propane/Propylene Diffusion in Zeolites: Framework Dynamics. *Journal of Physical Chemistry C*, **2009**, 113, 11246-11253	3.8	40
68	Quantum-chemistry calculations of hydrogen adsorption in MOF-5. *Physical Chemistry Chemical Physics*, **2009**, 11, 9250-8	3.6	25
67	Periodic DFT Calculation of the Energy of Ammonia Adsorption on Zeolite Brønsted Acid Sites to Support the Ammonia IRMS-TPD Experiment. *Chemistry Letters*, **2009**, 38, 354-355	1.7	17
66	Computational Study of Brønsted Acidity of Faujasite. Effect of the Al Content on the Infrared OH Stretching Frequencies. *Journal of Physical Chemistry C*, **2008**, 112, 19293-19301	3.8	23

65	A zeolitic structure (ITQ-34) with connected 9- and 10-ring channels obtained with phosphonium cations as structure directing agents. *Journal of the American Chemical Society*, **2008**, 130, 16482-3	16.4	99
64	Synthesis of the Ti-silicate Form of BEC Polymorph of Zeolite Assisted by Molecular Modeling. *Journal of Physical Chemistry C*, **2008**, 112, 19547-19554	3.8	52
63	A computational chemistry insight in the role of structure directing agents in the synthesis of zeolites. *Physical Chemistry Chemical Physics*, **2007**, 9, 1052-8	3.6	21
62	Gem-diamines as highly active organocatalysts for carbon–carbon bond formation. *Journal of Catalysis*, **2007**, 246, 136-146	7.3	54
61	Quantitative Measurements of Brønsted Acidity of Zeolites by Ammonia IRMS-TPD Method and Density Functional Calculation. *Chemistry Letters*, **2007**, 36, 1034-1035	1.7	23
60	Ammonia IRMS-TPD measurements and DFT calculation on acidic hydroxyl groups in CHA-type zeolites. *Physical Chemistry Chemical Physics*, **2007**, 9, 5980-7	3.6	47
59	Isomerization and disproportionation of m-xylene in a zeolite with 9- and 10-membered ring pores: Molecular dynamics and catalytic studies. *Journal of Catalysis*, **2006**, 242, 195-206	7.3	47
58	Computational study of 19F NMR spectra of double four ring-containing Si/Ge-zeolites. *ChemPhysChem*, **2006**, 7, 1092-9	3.2	39
57	Rings and strain in pure silica zeolites. *Journal of Physical Chemistry B*, **2006**, 110, 17949-59	3.4	27
56	Computational study of location and role of fluoride in zeolite structures. *Journal of Physical Chemistry B*, **2006**, 110, 23951-61	3.4	26
55	Further investigations into zeolite synthesis using flexible diquaternary alkylammonium ions (CnH2n+1)2HN+(CH2)5N+H(CnH2n+1)2 with n = 1–5 as structure-directing agents. *Microporous and Mesoporous Materials*, **2006**, 95, 366-371	5.3	2
54	Influence of pore dimension and sorption configuration on the heat of sorption of hexane on monodimensional siliceous zeolites. *Journal of Physical Chemistry B*, **2005**, 109, 23794-803	3.4	15
53	Pentacoordinated germanium in AST zeolite synthesised in fluoride media. A 19F NMR validated computational study. *Chemical Communications*, **2005**, 2357-9	5.8	19
52	Searching Organic Structure Directing Agents for the Synthesis of Specific Zeolitic Structures: An Experimentally Tested Computational Study. *Chemistry of Materials*, **2005**, 17, 545-552	9.6	44
51	Derivation of an Interatomic Potential for Fluoride-Containing Microporous Silicates and Germanates. *Chemistry of Materials*, **2005**, 17, 730-740	9.6	17
50	An attempt to predict and rationalize relative stabilities and preferential germanium location in Si/Ge zeolites. *Microporous and Mesoporous Materials*, **2005**, 82, 159-163	5.3	32
49	Dehydroaromatization of methane under non-oxidative conditions over bifunctional Mo/ITQ-2 catalysts. *Catalysis Today*, **2005**, 107-108, 676-684	5.3	42
48	A new synthesis method for the preparation of ITQ-7 zeolites and the characterisation of the resulting materials. *Comptes Rendus Chimie*, **2005**, 8, 369-378	2.7	18

47	A multisite molecular mechanism for Baeyer-Villiger oxidations on solid catalysts using environmentally friendly H2O2 as oxidant. *Chemistry - A European Journal*, **2005**, 11, 6905-15	4.8	80
46	An study of cyclohexylpyrrolidine-derived quaternary organic cations as structure directing agents for synthesis of zeolites. *Studies in Surface Science and Catalysis*, **2004**, 154, 265-274	1.8	0
45	Xylene isomerization and aromatic alkylation in zeolites NU-87, SSZ-33, and ZSM-5: molecular dynamics and catalytic studies. *Journal of Catalysis*, **2004**, 227, 227-241	7.3	86
44	Synthesis, characterization, and framework heteroatom localization in ITQ-21. *Journal of the American Chemical Society*, **2004**, 126, 13414-23	16.4	54
43	Effect of the Germanium Incorporation in the Synthesis of EU-1, ITQ-13, ITQ-22, and ITQ-24 Zeolites. *Journal of Physical Chemistry B*, **2004**, 108, 8830-8835	3.4	62
42	Topological and geometrical characterization of zeotypes with a free software code called zeotsites: The case study of germanium location in octadecasil. *Studies in Surface Science and Catalysis*, **2004**, 1261-1266	1.8	2
41	A new synthesis route of the tridirectional 12 ring channel zeolite ITQ-7. *Studies in Surface Science and Catalysis*, **2004**, 481-488	1.8	4
40	Ordinary Diffusion and Single File Diffusion in Zeolites with Monodimensional Channels. Benzene and n-Butane in ITQ-4 and L Zeolites. *Topics in Catalysis*, **2003**, 24, 7-12	2.3	6
39	On the shape selective acylation of 2-methoxynaphthalene over polymorph C of Beta (ITQ-17). *Journal of Catalysis*, **2003**, 217, 406-416	7.3	43
38	Derivation of an Interatomic Potential for Germanium- and Silicon-Containing Zeolites and Its Application to the Study of the Structures of Octadecasil, ASU-7, and ASU-9 Materials. *Chemistry of Materials*, **2003**, 15, 1788-1796	9.6	44
37	A software tool for the topological and geometrical characterization of three-dimensional frameworks. *Computational Materials Science*, **2003**, 28, 77-84	3.2	3
36	Computational and Experimental Approach to the Role of Structure-Directing Agents in the Synthesis of Zeolites: The Case of Cyclohexyl Alkyl Pyrrolidinium Salts in the Synthesis of EU-1, ZSM-11, and ZSM-12 Zeolites. *Journal of Physical Chemistry B*, **2003**, 107, 5432-5440	3.4	72
35	Preferential Location of Ge Atoms in Polymorph C of Beta Zeolite (ITQ-17) and Their Structure-Directing Effect: A Computational, XRD, and NMR Spectroscopic Study. *Angewandte Chemie*, **2002**, 114, 4916-4920	3.6	17
34	Preferential location of Ge atoms in polymorph C of beta zeolite (ITQ-17) and their structure-directing effect: a computational, XRD, and NMR spectroscopic study. *Angewandte Chemie - International Edition*, **2002**, 41, 4722-6	16.4	123
33	Influence of the Intermolecular Interactions on the Mobility of Heptane in the Supercages of MCM-22 Zeolite. A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2002**, 106, 956-962	3.4	19
32	On the Preferential Location of Al and Proton Siting in Zeolites: A Computational and Infrared Study. *Journal of Physical Chemistry B*, **2002**, 106, 701-708	3.4	73
31	Simultaneous hydrogenation and ring opening of aromatics for diesel upgrading on Pt/zeolite catalysts. The influence of zeolite pore topology and reactant on catalyst performance. *Studies in Surface Science and Catalysis*, **2002**, 142, 1015-1022	1.8	13
30	ZeoTsites: a code for topological and crystallographic tetrahedral sites analysis in zeolites and zeotypes. *Microporous and Mesoporous Materials*, **2001**, 43, 27-40	5.3	44

29	Al-ITQ-7, a Shape-Selective Zeolite for Acylation of 2-Methoxynaphthalene. *Journal of Catalysis*, **2001**, 197, 81-90	7.3	46
28	A Computational Study on the Templating Ability of the Trispyrrolidinium Cation in the Synthesis of ZSM-18 Zeolite. *Chemistry of Materials*, **2001**, 13, 4520-4526	9.6	36
27	On the Mechanism of Alkane Isomerisation (Isodewaxing) with Unidirectional 10-Member Ring Zeolites. A Molecular Dynamics and Catalytic Study. *Journal of Catalysis*, **2000**, 195, 227-236	7.3	67
26	Preferential Siting of Bridging Hydroxyls and Their Different Acid Strengths in the Two-Channel System of MCM-22 Zeolite. *Journal of Physical Chemistry B*, **2000**, 104, 4349-4354	3.4	52
25	Molecular Dynamics of C7 Hydrocarbon Diffusion in ITQ-2. The Benefit of Zeolite Structures Containing Accessible Pockets. *Journal of Physical Chemistry B*, **2000**, 104, 416-422	3.4	25
24	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	3.6	15
23	Relation between structure and Lewis acidity of Ti-Beta and TS-1 zeolites. *Chemical Physics Letters*, **1999**, 302, 447-453	2.5	49
22	Catalytic Activity of Proton Sponge: Application to Knoevenagel Condensation Reactions. *Journal of Catalysis*, **1999**, 183, 14-23	7.3	66
21	Diffusion of a para- and ortho-xylene mixture in CIT-1 zeolite: a molecular dynamics study. *Topics in Catalysis*, **1999**, 9, 215-224	2.3	9
20	Influence of short- and long-range factors in the Brønsted acidity of MCM-22 zeolite. *Chemical Communications*, **1999**, 2163-2164	5.8	4
19	Rationalisation of the IR stretching frequencies of Brønsted acid centres in microporous solids. *Chemical Communications*, **1999**, 349-350	5.8	20
18	Diffusion of Octane in Silicalite: A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **1999**, 103, 11007-11015	3.4	16
17	Diffusion of Benzene and Propylene in MCM-22 Zeolite. A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **1999**, 103, 5187-5196	3.4	76
16	Modelling of Brønsted acidity in AFI and CHA zeotypes. *Journal of the Chemical Society, Faraday Transactions*, **1998**, 94, 3049-3058		63
15	Diffusion of Linear and Branched C7 Paraffins in ITQ-1 Zeolite. A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **1998**, 102, 7085-7090	3.4	21
14	Selective Diffusion of C8 Aromatics in a 10 and 12 MR Zeolite. A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **1998**, 102, 3198-3209	3.4	50
13	Activation of Molecules in Confined Spaces: An Approach to Zeolite–Guest Supramolecular Systems. *Journal of Physical Chemistry B*, **1997**, 101, 4575-4582	3.4	68
12	Modeling of Silicon Substitution in SAPO-5 and SAPO-34 Molecular Sieves. *Journal of Physical Chemistry B*, **1997**, 101, 5249-5262	3.4	164

11	On the Incorporation of Buckminsterfullerene C60 in the Supercages of Zeolite Y. *Journal of Physical Chemistry B*, **1997**, 101, 10184-10190	3.4	26
10	Introductory Lecture Computer modelling as a technique in solid state chemistry. *Faraday Discussions*, **1997**, 106, 1-40	3.6	38
9	Modelling of structure, sorption, synthesis and reactivity in catalytic systems1Communication presented at the First Francqui Colloquium, Brussels, 19?0 February 1996.1. *Journal of Molecular Catalysis A*, **1997**, 115, 431-448		11
8	Mechanisms of silicon incorporation in aluminophosphate molecular sieves. *Journal of Molecular Catalysis A*, **1997**, 119, 349-356		52
7	Quantum chemistry calculations on the effect of electron confinement upon the frontier molecular orbitals of ethylene and benzene in sodalite. Implications on reactivity. *Chemical Physics Letters*, **1997**, 264, 565-572	2.5	9
6	Computer Simulation of Catalytic Systems **1997**, 5-29		
5	Structure and Stability of Silica Species in SAPO Molecular Sieves. *The Journal of Physical Chemistry*, **1996**, 100, 6722-6730		99
4	Space group symmetry and Al□P bond angles in AlPO4-5. *Journal of Materials Chemistry*, **1996**, 6, 1837-1842		29
3	A quantum-chemical study of para/ortho-toluene alkylation by adsorbed methoxy species on zeolites. *Journal of Molecular Catalysis A*, **1995**, 100, 75-85		16
2	Quantum-chemistry calculations of surface complex and orbital control in para/ortho toluene alkylation catalyzed by big pore zeolites. *Studies in Surface Science and Catalysis*, **1994**, 84, 2171-2178	1.8	10
1	Molecular orbital calculation of the soft-hard acidity of zeolites and its catalytic implications. *Journal of Catalysis*, **1992**, 136, 521-530	7.3	31