Claudio M Zicovich-Wilson

List of Publications by Year
in descending order

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137	11,039	47006	30087
papers	citations	47	103
		h-index	g-index

142	142	142	8509
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantumâ€mechanical condensed matter simulations with CRYSTAL. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1360.	14.6	1,277
2	Long-range exchange limit and dispersion in pure silica zeolites. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	3
3	Full Mechanism of Zeolite Dealumination in Aqueous Strong Acid Medium: Ab Initio Periodic Study on H-Clinoptilolite. Journal of Physical Chemistry C, 2017, 121, 2652-2660.	3.1	20
4	The A-center defect in diamond: quantum mechanical characterization through the infrared spectrum. Physical Chemistry Chemical Physics, 2017, 19, 14478-14485.	2.8	16
5	Nuclearâ€relaxed elastic and piezoelectric constants of materials: Computational aspects of two quantumâ€mechanical approaches. Journal of Computational Chemistry, 2017, 38, 257-264.	3.3	16
6	Antiferromagnetic vs. non-magnetic Îµ phase of solid oxygen. Periodic density functional theory studies using a localized atomic basis set and the role of exact exchange. Physical Chemistry Chemical Physics, 2017, 19, 2826-2833.	2.8	8
7	The V + I defects in diamond: An ab initio investigation of the electronic structure, of the Raman and IR spectra, and of their possible recombination. Journal of Chemical Physics, 2016, 145, 184701.	3.0	9
8	Serpentine polymorphism: a quantitative insight from first-principles calculations. CrystEngComm, 2016, 18, 4412-4419.	2.6	24
9	Hirshfeld-I charges in linear combination of atomic orbitals periodic calculations. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	16
10	Infrared and Raman spectroscopic features of the self-interstitial defect in diamond from exact-exchange hybrid DFT calculations. Physical Chemistry Chemical Physics, 2016, 18, 21288-21295.	2.8	31
11	Direct Piezoelectric Tensor of 3D Periodic Systems through a Coupled Perturbed Hartreeâ€“Fock/Kohnâ€“Sham Method. Zeitschrift Fur Physikalische Chemie, 2016, 230, 719-736.	2.8	11
12	The influence of the DFT approach on the structure and relative stability of models for cellulose I allomorphs. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	7
13	Solid oxygen<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î¶</mml:mi></mml:math>phase and its transition from<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>É›</mml:mi></mml:math>phase at extremely high pressure: A first-principles analysis. Physical Review B, 2015, 92, .	3.2	15
14	Katoite under pressure: an ab initio investigation of its structural, elastic and vibrational properties sheds light on the phase transition. Physical Chemistry Chemical Physics, 2015, 17, 2660-2669.	2.8	16
15	Understanding the Îµ and Î¶ High-Pressure Solid Phases of Oxygen. Systematic Periodic Density Functional Theory Studies Using Localized Atomic Basis. Journal of Chemical Theory and Computation, 2015, 11, 1195-1205.	5.3	15
16	Chemical interaction of water molecules with framework Al in acid zeolites: a periodic ab initio study on H-clinoptilolite. Physical Chemistry Chemical Physics, 2015, 17, 23657-23666.	2.8	9
17	On the Raman and infrared vibrational spectra of the É› and Î¶ phases of oxygen. Systematic DFT studies with localized basis sets. Chemical Physics Letters, 2015, 638, 82-86.	2.6	7
18	The role of long-range van der Waals forces in the relative stability of SiO 2 -zeolites. Chemical Physics Letters, 2015, 619, 109-114.	2.6	27

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19	C<scp>RYSTAL14</scp>: A program for the ab initio investigation of crystalline solids. International Journal of Quantum Chemistry, 2014, 114, 1287-1317.	2.0	1,151
20	On the full exploitation of symmetry in periodic (as well as molecular) self-consistent-field ab initio calculations. Journal of Chemical Physics, 2014, 141, 104108.	3.0	21
21	Exploitation of symmetry in periodic Self-Consistent-Field ab initio calculations: application to large three-dimensional compounds. Science China Chemistry, 2014, 57, 1418-1426.	8.2	4
22	Structural, electronic and energetic properties of giant icosahedral fullerenes up to C6000: insights from an ab initio hybrid DFT study. Physical Chemistry Chemical Physics, 2014, 16, 13390-13401.	2.8	30
23	Periodic Quantum Chemical Studies on Anhydrous and Hydrated Acid Clinoptilolite. Journal of Physical Chemistry A, 2014, 118, 5779-5789.	2.5	11
24	Synthesis of Aluminosilicate Natrolites and Control of Their Tetrahedral Atom Ordering. Chemistry of Materials, 2014, 26, 3361-3363.	6.7	15
25	The molecular and electronic structure of poly-[2,7-(benzo[2,1;3,4-bâ€²]dithiophene)-alt-2,2â€²-(3,3â€²-didodecyl-5,5â€²-bithiophenyl)] (PBTT): A periodic DFT approach. Chemical Physics Letters, 2014, 607, 47-51.	2.6	1
26	Electronic Charge Density Analysis of Li-Doped Polyacetylene: Molecular vs Periodic Descriptions and Nature of Li-to-Chain Bonding. Journal of Physical Chemistry B, 2013, 117, 725-730.	2.6	1
27	Boronate Ligands in Materials: Determining Their Local Environment by Using a Combination of IR/Solidâ€State NMR Spectroscopies and DFT Calculations. Chemistry - A European Journal, 2013, 19, 880-891.	3.3	19
28	The electronic structure of MgO nanotubes. An ab initio quantum mechanical investigation. Physical Chemistry Chemical Physics, 2013, 15, 13296.	2.8	10
29	Hostâ€“Guest Stabilization of a Zeolite Strained Framework: In Situ Transformation of Zeolite MTW into the Less Dense and More Strained ITW. Chemistry of Materials, 2013, 25, 729-738.	6.7	30
30	Raman Spectrum of Pyrope Garnet. A Quantum Mechanical Simulation of Frequencies, Intensities, and Isotope Shifts. Journal of Physical Chemistry A, 2013, 117, 11464-11471.	2.5	25
31	On the use of symmetry in SCF calculations. The case of fullerenes and nanotubes. AIP Conference Proceedings, 2012, , .	0.4	9
32	Exceptionally Low Shear Modulus in a Prototypical Imidazole-Based Metal-Organic Framework. Physical Review Letters, 2012, 108, 095502.	7.8	210
33	Coupled perturbed HF/KS calculation of the dielectric constant of crystalline systems. The case of six members of the garnet family. , 2012, , .		1
34	Zeolite Synthesis in Fluoride Media: Structure Direction toward ITW by Small Methylimidazolium Cations. Journal of the American Chemical Society, 2012, 134, 2255-2263.	13.7	56
35	Electronic structure, dielectric properties and infrared vibrational spectrum of fayalite: An ab initio simulation with an allâ€electron Gaussian basis set and the B3LYP functional. International Journal of Quantum Chemistry, 2012, 112, 2098-2108.	2.0	20
36	Beyond Wigner's theorems: The role of symmetry equivalences in quantum systems. International Journal of Quantum Chemistry, 2012, 112, 3543-3551.	2.0	3

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37	Adjusting framework ionicity to favour crystallisation of zeolites with strained structural units. Periodic quantum chemical studies. Catalysis Science and Technology, 2011, 1, 868.	4.1	8
38	Comparative Study on the Performance of Hybrid DFT Functionals in Highly Correlated Oxides: The Case of CeO₂and Ce₂O₃. Journal of Chemical Theory and Computation, 2011, 7, 56-65.	5.3	125
39	Properties of Carbon Nanotubes: An ab Initio Study Using Large Gaussian Basis Sets and Various DFT Functionals. Journal of Physical Chemistry C, 2011, 115, 8876-8885.	3.1	42
40	Initial structure of cetyltrimethylammonium bromide micelles in aqueous solution from molecular dynamics simulations. Soft Matter, 2011, 7, 8508.	2.7	29
41	Physico-Chemical Features of Aluminum Hydroxides As Modeled with the Hybrid B3LYP Functional and Localized Basis Functions. Journal of Physical Chemistry C, 2011, 115, 13107-13134.	3.1	50
42	The IR vibrational properties of six members of the garnet family: A quantum mechanical ab initio study. American Mineralogist, 2011, 96, 1787-1798.	1.9	28
43	Structure and Xâ€ray spectrum of crystalline poly(3â€hexylthiophene) from DFTâ€van der Waals calculations. Physica Status Solidi (B): Basic Research, 2011, 248, 1360-1368.	1.5	65
44	On the use of symmetry in the ab initio quantum mechanical simulation of nanotubes and related materials. Journal of Computational Chemistry, 2010, 31, 855-862.	3.3	48
45	A fundamental connection between symmetry and spatial localization properties of basis sets. Theoretical Chemistry Accounts, 2010, 126, 165-175.	1.4	8
46	Catalytic Reaction Mechanism of Mnâ€Doped Nanoporous Aluminophosphates for the Aerobic Oxidation of Hydrocarbons. Chemistry - A European Journal, 2010, 16, 13638-13645.	3.3	37
47	Flexibility in a Metalâ€“Organic Framework Material Controlled by Weak Dispersion Forces: The Bistability of MILâ€53(Al). Angewandte Chemie, 2010, 122, 7663-7665.	2.0	35
48	Flexibility in a Metalâ€“Organic Framework Material Controlled by Weak Dispersion Forces: The Bistability of MILâ€53(Al). Angewandte Chemie - International Edition, 2010, 49, 7501-7503.	13.8	158
49	Magnetic interactions and electronic structure of uvarovite and andradite garnets. An ab initio allâ€electron simulation with the CRYSTAL06 program. International Journal of Quantum Chemistry, 2010, 110, 338-351.	2.0	14
50	Anatase(001) 3 ML Nanotubes, The First TiO₂ Nanotube With Negative Strain Energies: A DFT Prediction. Journal of Physical Chemistry Letters, 2010, 1, 2854-2857.	4.6	41
51	Comment on â€œAccurate Hartree-Fock energy of extended systems using large Gaussian basis setsâ€• Physical Review B, 2010, 81, .	3.2	13
52	Mechanism of F^{â^'} Elimination from Zeolitic D4R Units: A Periodic B3LYP Study on the Octadecasil Zeolite. Journal of Physical Chemistry C, 2010, 114, 2989-2995.	3.1	16
53	In SituTransformation of TON Silica Zeolite into the Less Dense ITW: Structure-Direction Overcoming Framework Instability in the Synthesis of SiO₂Zeolites. Journal of the American Chemical Society, 2010, 132, 3461-3471.	13.7	53
54	Search and Characterization of Transition State Structures in Crystalline Systems Using Valence Coordinates. Journal of Chemical Theory and Computation, 2010, 6, 1341-1350.	5.3	19

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55	Periodic density functional theory calculations for 3-dimensional polyacetylene with empirical dispersion terms. Physical Chemistry Chemical Physics, 2010, 12, 3289.	2.8	23
56	Role of dispersive interactions in the CO adsorption on MgO(001): periodic B3LYP calculations augmented with an empirical dispersion term. Physical Chemistry Chemical Physics, 2010, 12, 6382.	2.8	60
57	Ab initio modeling of layered materials with the CRYSTAL code: an overview. Zeitschrift FÃ¼r Kristallographie, 2009, 224, 241-250.	1.1	8
58	Ab initio quantumâ€mechanical simulation of the Raman spectrum of grossular. Journal of Raman Spectroscopy, 2009, 40, 416-418.	2.5	19
59	On the Interaction between Silica Surfaces and Surfactants. A 2D Periodic B3LYP Investigation. Journal of Physical Chemistry C, 2009, 113, 13309-13316.	3.1	6
60	Periodic DFT modeling of bulk and surface properties of MgCl2. Physical Chemistry Chemical Physics, 2009, 11, 6525.	2.8	54
61	Periodic density functional theory studies of Li-doped polythiophene: Dependence of electronic and structural properties on dopant concentration. Journal of Chemical Physics, 2009, 130, 164904.	3.0	16
62	Ab initio modeling of protein/biomaterial interactions: competitive adsorption between glycine and water onto hydroxyapatite surfaces. Physical Chemistry Chemical Physics, 2009, 11, 9005.	2.8	40
63	Role of dispersive interactions in layered materials: a periodic B3LYP and B3LYP-D* study of Mg(OH)2, Ca(OH)2 and kaolinite. Journal of Materials Chemistry, 2009, 19, 2564.	6.7	75
64	Ab initio simulation of the IR spectra of pyrope, grossular, and andradite. Journal of Computational Chemistry, 2008, 29, 2268-2278.	3.3	84
65	B3LYP augmented with an empirical dispersion term (B3LYP-D*) as applied to molecular crystals. CrystEngComm, 2008, 10, 405-410.	2.6	775
66	Ab Initio Modeling of Protein/Biomaterial Interactions: Glycine Adsorption at Hydroxyapatite Surfaces. Journal of the American Chemical Society, 2008, 130, 16181-16183.	13.7	97
67	Periodic Density Functional Theory Calculations for Na-doped Quasi-one-dimensional Polyacetylene Chains. Journal of Physical Chemistry C, 2008, 112, 9493-9500.	3.1	8
68	Ab-initioquantum mechanical study of akdalaite (5Al₂O₃Â·) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 227 012013.	0.4	12
69	Two points of view to look at symmetry. Journal of Physics: Conference Series, 2008, 117, 012030.	0.4	4
70	Ab-initio thermal physics and Cr-isotopic fractionation of MgCr2O4. American Mineralogist, 2007, 92, 98-108.	1.9	8
71	Structure, Vibrational Analysis, and Insights into Hostâ^'Guest Interactions in As-Synthesized Pure Silica ITQ-12 Zeolite by Periodic B3LYP Calculations. Journal of the American Chemical Society, 2007, 129, 11512-11523.	13.7	55
72	Uniplanar Orientations as a Tool To Assign Vibrational Modes of Polymer Chain. Macromolecules, 2007, 40, 3895-3897.	4.8	33

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73	Periodic DFT Studies of AlPO-11:â€‰ The Role of Hydration on Structural Properties. Journal of Physical Chemistry C, 2007, 111, 9664-9670.	3.1	9
74	Ab Initio Investigation of Structure and Cohesive Energy of Crystalline Urea. Journal of Physical Chemistry B, 2007, 111, 26-33.	2.6	87
75	Ab initio vibrational spectra and dielectric properties of carbonates: magnesite, calcite and dolomite. Theoretical Chemistry Accounts, 2007, 117, 991-1000.	1.4	108
76	Influence of the exchange-correlation functional in all-electron calculations of the vibrational frequencies of corundum (Î±-Al2O3). International Journal of Quantum Chemistry, 2006, 106, 1703-1714.	2.0	71
77	A quantum-mechanical study of the vinyl fluoride adsorbed on the rutile TiO2(110) surface. Surface Science, 2006, 600, 305-317.	1.9	43
78	Symmetry-adapted Localized Wannier Functions Suitable for Periodic Local Correlation Methods. Theoretical Chemistry Accounts, 2006, 116, 726-733.	1.4	49
79	Periodic Hartree-Fock and density functional theory calculations for Li-doped polyacetylene chains. Journal of Chemical Physics, 2006, 124, 244703.	3.0	14
80	Ab InitioStudy of the Vibrational Spectrum and Related Properties of Crystalline Compounds; the Case of CaCO3Calcite. Zeitschrift Fur Physikalische Chemie, 2006, 220, 893-912.	2.8	168
81	The constrained space orbital variation analysis for periodic ab initio calculations. Journal of Chemical Physics, 2006, 124, 194105.	3.0	7
82	Phonon vibrational frequencies and elastic properties of solid SrFCl. An ab initio study. European Physical Journal B, 2005, 43, 453-461.	1.5	26
83	Vibration Frequencies of Mg3Al2Si3O12 Pyrope. An ab initio Study with the CRYSTAL Code.. ChemInform, 2005, 36, no.	0.0	2
84	Local-MP2 electron correlation method for nonconducting crystals. Journal of Chemical Physics, 2005, 122, 094113.	3.0	182
85	CRYSTAL: a computational tool for the ab initio study of the electronic properties of crystals. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.8	824
86	Carbon monoxide adsorption on alkali and proton-exchanged chabazite: anab-initioperiodic study using the CRYSTAL code. Molecular Physics, 2005, 103, 2559-2571.	1.7	32
87	Vibration Frequencies of Mg3Al2Si3O12 Pyrope. An ab Initio Study with the CRYSTAL Code. Journal of Physical Chemistry B, 2005, 109, 6146-6152.	2.6	142
88	The Isobutyleneâ"Isobutane Alkylation Process in Liquid HF Revisited. Journal of Physical Chemistry B, 2005, 109, 12946-12955.	2.6	10
89	The vibrational spectrum of calcite (CaCO3): an ab initio quantum-mechanical calculation. Physics and Chemistry of Minerals, 2004, 31, 559-564.	0.8	182
90	The calculation of the vibrational frequencies of crystalline compounds and its implementation in the CRYSTAL code. Journal of Computational Chemistry, 2004, 25, 888-897.	3.3	796

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91	Calculation of the vibration frequencies of ?-quartz: The effect of Hamiltonian and basis set. Journal of Computational Chemistry, 2004, 25, 1873-1881.	3.3	451
92	Can Cu+-Exchanged Zeolites Store Molecular Hydrogen? An ab initio Periodic Study Compared with Low-Temperature FTIR.. ChemInform, 2004, 35, no.	0.0	0
93	Vibrational spectrum of brucite, Mg(OH)2: a periodic ab initio quantum mechanical calculation including OH anharmonicity. Chemical Physics Letters, 2004, 396, 308-315.	2.6	142
94	In Situ Disorderâ^'Order Transformation in Synthetic Gallosilicate Zeolites with the NAT Topology. Journal of the American Chemical Society, 2004, 126, 13742-13751.	13.7	45
95	Can Cu+-Exchanged Zeolites Store Molecular Hydrogen? An Ab-Initio Periodic Study Compared with Low-Temperature FTIR. Journal of Physical Chemistry B, 2004, 108, 8278-8286.	2.6	91
96	Periodic ab Initio Study of the Electronic Structure of Î±-Al2O3and AlN(w) Surfaces Based on Localized Wannier Functions. Journal of Physical Chemistry B, 2004, 108, 7316-7322.	2.6	6
97	Structural, Electronic, and Vibrational Properties of the Tiâ^'Oâ^'Ti Quantum Wires in the Titanosilicate ETS-10. Journal of Physical Chemistry B, 2004, 108, 1328-1336.	2.6	79
98	DFT Cluster Calculations for Alkali Cation-Exchanged Zeolites Interacting with Ethylchloride and HCl. Journal of Physical Chemistry B, 2004, 108, 10658-10662.	2.6	12
99	Modeling Soot and Its Functionalization under Atmospheric or Combustion Conditions by Density Functional Theory within Molecular (Polycyclic-Aromatic-Hydrocarbon-like) and Periodic Methodologies. Journal of Physical Chemistry B, 2004, 108, 3215-3223.	2.6	35
100	Electronic structure characterization of six semiconductors through their localized Wannier functions. Physical Chemistry Chemical Physics, 2003, 5, 5319.	2.8	6
101	Infrared Investigation of Fluoride Occluded in Double Four-Member Rings in Zeolites. Journal of Physical Chemistry B, 2002, 106, 2796-2800.	2.6	23
102	Preferential Location of Ge in the Double Four-Membered Ring Units of ITQ-7 Zeolite. Journal of Physical Chemistry B, 2002, 106, 2634-2642.	2.6	228
103	Characterization of the electronic structure of crystalline compounds through their localized Wannier functions. Journal of Chemical Physics, 2002, 116, 1120-1127.	3.0	87
104	Polarization properties of ZnO and BeO:â€ƒAnab initiostudy through the Berry phase and Wannier functions approaches. Physical Review B, 2001, 65, .	3.2	213
105	Naphthalene Included within All-Silica Zeolites:Â Influence of the Host on the Naphthalene Photophysics. Journal of Physical Chemistry B, 2001, 105, 9973-9979.	2.6	63
106	Influence of the Local Geometry of Zeolite Active Sites and Olefin Size on the Stability of Alkoxide Intermediates. Journal of Physical Chemistry B, 2001, 105, 11169-11177.	2.6	66
107	Cluster and Periodic Calculations of the Ethene Protonation Reaction Catalyzed by theta-1 Zeolite: Influence of Method, Model Size, and Structural Constraints. Chemistry - A European Journal, 2001, 7, 1295-1303.	3.3	28
108	A general method to obtain well localized Wannier functions for composite energy bands in linear combination of atomic orbital periodic calculations. Journal of Chemical Physics, 2001, 115, 9708-9719.	3.0	191

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109	Well localized crystalline orbitals obtained from Bloch functions:â€ƒThe case ofKNbO3. Physical Review B, 2001, 64, .	3.2	50
110	H-Chabazite with variable Si/Al ratio: stability and OH vibrational frequency computed in a periodic LCAO B3-LYP approach. Chemical Physics Letters, 2000, 318, 247-255.	2.6	52
111	Charge distribution in NaY zeolite from charge-transfer molecular dynamics. Chemical Physics Letters, 2000, 327, 224-229.	2.6	9
112	Modifying the Catalytic Activity of Ti-Zeolites by Isomorphic Substitution of Si by Ge Atoms. A Periodic Quantum-Chemical Study. Journal of Physical Chemistry B, 2000, 104, 4134-4140.	2.6	28
113	A periodic Hartreeâ€“Fock study of Na adsorption on the TiO2(110) rutile surface. Chemical Physics Letters, 1999, 303, 111-116.	2.6	18
114	High-pressure decomposition of MCr 2 O 4 spinels (M=Mg, Mn, Zn) by ab initio methods. Physics and Chemistry of Minerals, 1999, 26, 389-395.	0.8	45
115	Periodic B3-LYP calculations on H-Edingtonites, both alone and interacting with acetylene. Physical Chemistry Chemical Physics, 1999, 1, 545-553.	2.8	31
116	Cluster and periodic ab initio study of the ethane-ethene hydride transfer reaction catalyzed by acid chabazite. Is the cluster model able to describe accurately the hostâ€“guest interactions?. Physical Chemistry Chemical Physics, 1999, 1, 537-543.	2.8	35
117	Interaction of Ti-Zeolites with Water. A Periodic ab Initio Study. Journal of Physical Chemistry B, 1999, 103, 988-994.	2.6	37
118	A periodic ab initio study of the structure and relative stability of silica polymorphs. Chemical Physics Letters, 1998, 292, 394-402.	2.6	74
119	On the use of symmetry-adapted crystalline orbitals in SCF-LCAO periodic calculations. I. The construction of the symmetrized orbitals. , 1998, 67, 299-309.		53
120	On the use of symmetry-adapted crystalline orbitals in SCF-LCAO periodic calculations. II. Implementation of the self-consistent-field scheme and examples. , 1998, 67, 311-320.		27
121	Trapped-hole centres containing lithium and sodium in MgO, CaO and SrO. An ab initio supercell study. Journal of Physics and Chemistry of Solids, 1998, 59, 1119-1124.	4.0	20
122	Titanium-Containing Zeolites. A Periodic ab Initio Hartreeâ˜'Fock Characterization. Journal of Physical Chemistry B, 1998, 102, 1411-1417.	2.6	64
123	On the structure and stability ofTi-zeolites. A comparison of cluster and periodicab initio calculations. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1997, 19, 1785-1790.	0.4	5
124	Periodic ab initio study of the oxidizing sites in Ti-containing zeolites. Journal of Molecular Catalysis A, 1997, 119, 449-458.	4.8	20
125	Periodic ab initio study of silico-faujasite. Chemical Physics Letters, 1997, 277, 227-233.	2.6	16
126	Semiempirical Hamiltonians for spatially confined ?-electron systems. , 1996, 60, 971-981.		8

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127	Atoms and molecules in cavities: A method for study of spatial confinement effects. International Journal of Quantum Chemistry, 1995, 54, 61-72.	2.0	19
128	27Al and 29Si MAS NMR Study of Zeolite MCM-22. The Journal of Physical Chemistry, 1995, 99, 7002-7008.	2.9	87
129	Formation of Surface Methoxy Groups on H-Zeolites from Methanol. A Quantum Chemical Study. The Journal of Physical Chemistry, 1995, 99, 13224-13231.	2.9	88
130	Electronic Confinement of Molecules in Microscopic Pores. A New Concept Which Contributes to the Explanation of the Catalytic Activity of Zeolites. The Journal of Physical Chemistry, 1994, 98, 10863-10870.	2.9	138
131	Orbital-controlled reactions catalysed by zeolites: Electrophilic alkylation of aromatics. Journal of Physical Organic Chemistry, 1994, 7, 364-370.	1.9	13
132	Spatially confined simple quantum mechanical systems. International Journal of Quantum Chemistry, 1994, 50, 429-444.	2.0	65
133	Acid softness and hardness in large-pore zeolites as a determinant parameter to control selectivity in orbital-controlled reactions. Journal of the American Chemical Society, 1994, 116, 134-142.	13.7	55
134	A simple proof for the formula to get symmetrized powers of group representations. International Journal of Quantum Chemistry, 1993, 47, 319-323.	2.0	1
135	Ab initio molecular orbital calculations of the protonation of propylene and isobutene by acidic hydroxyl groups of isomorphously substituted zeolites. The Journal of Physical Chemistry, 1993, 97, 13713-13719.	2.9	105
136	Molecular orbital calculation of the soft-hard acidity of zeolites and its catalytic implications. Journal of Catalysis, 1992, 136, 521-530.	6.2	31
137	Theoretical EHT study of oxidative coupling of methane on pure MgO and MgO doped with Li and Na. Journal of Molecular Catalysis, 1991, 64, 191-200.	1.2	11