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	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
3	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
4	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
5	B3LYP augmented with an empirical dispersion term (B3LYP-D*) as applied to molecular crystals. CrystEngComm, 2008, 10, 405-410.	2.6	775
6	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
7	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
8	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
9	Exceptionally Low Shear Modulus in a Prototypical Imidazole-Based Metal-Organic Framework. Physical Review Letters, 2012, 108, 095502.	7.8	210
10	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
11	The vibrational spectrum of calcite (CaCO3): an ab initio quantum-mechanical calculation. Physics and Chemistry of Minerals, 2004, 31, 559-564.	0.8	182
12	Local-MP2 electron correlation method for nonconducting crystals. Journal of Chemical Physics, 2005, 122, 094113.	3.0	182
13	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
14	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
15	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
16	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
17	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
18	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

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19	Ab initio vibrational spectra and dielectric properties of carbonates: magnesite, calcite and dolomite. Theoretical Chemistry Accounts, 2007, 117, 991-1000.	1.4	108
20	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
21	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
22	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
23	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
24	27Al and 29Si MAS NMR Study of Zeolite MCM-22. The Journal of Physical Chemistry, 1995, 99, 7002-7008.	2.9	87
25	Characterization of the electronic structure of crystalline compounds through their localized Wannier functions. Journal of Chemical Physics, 2002, 116, 1120-1127.	3.0	87
26	Ab Initio Investigation of Structure and Cohesive Energy of Crystalline Urea. Journal of Physical Chemistry B, 2007, 111, 26-33.	2.6	87
27	Ab initio simulation of the IR spectra of pyrope, grossular, and andradite. Journal of Computational Chemistry, 2008, 29, 2268-2278.	3.3	84
28	Structural, Electronic, and Vibrational Properties of the Tiâˆ’Oâˆ’Ti Quantum Wires in the Titanosilicate ETS-10. Journal of Physical Chemistry B, 2004, 108, 1328-1336.	2.6	79
29	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
30	A periodic ab initio study of the structure and relative stability of silica polymorphs. Chemical Physics Letters, 1998, 292, 394-402.	2.6	74
31	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
32	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
33	Spatially confined simple quantum mechanical systems. International Journal of Quantum Chemistry, 1994, 50, 429-444.	2.0	65
34	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
35	Titanium-Containing Zeolites. A Periodic ab Initio Hartreeâˆ’Fock Characterization. Journal of Physical Chemistry B, 1998, 102, 1411-1417.	2.6	64
36	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

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37	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
38	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
39	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
40	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
41	Periodic DFT modeling of bulk and surface properties of MgCl2. Physical Chemistry Chemical Physics, 2009, 11, 6525.	2.8	54
42	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
43	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
44	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
45	Well localized crystalline orbitals obtained from Bloch functions:â€ƒThe case ofKNbO3. Physical Review B, 2001, 64, .	3.2	50
46	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
47	Symmetry-adapted Localized Wannier Functions Suitable for Periodic Local Correlation Methods. Theoretical Chemistry Accounts, 2006, 116, 726-733.	1.4	49
48	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
49	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
50	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
51	A quantum-mechanical study of the vinyl fluoride adsorbed on the rutile TiO2(110) surface. Surface Science, 2006, 600, 305-317.	1.9	43
52	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
53	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
54	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

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55	Interaction of Ti-Zeolites with Water. A Periodic ab Initio Study. Journal of Physical Chemistry B, 1999, 103, 988-994.	2.6	37
56	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
57	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
58	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
59	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
60	Uniplanar Orientations as a Tool To Assign Vibrational Modes of Polymer Chain. Macromolecules, 2007, 40, 3895-3897.	4.8	33
61	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
62	Molecular orbital calculation of the soft-hard acidity of zeolites and its catalytic implications. Journal of Catalysis, 1992, 136, 521-530.	6.2	31
63	Periodic B3-LYP calculations on H-Edingtonites, both alone and interacting with acetylene. Physical Chemistry Chemical Physics, 1999, 1, 545-553.	2.8	31
64	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
65	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
66	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
67	Initial structure of cetyltrimethylammonium bromide micelles in aqueous solution from molecular dynamics simulations. Soft Matter, 2011, 7, 8508.	2.7	29
68	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
69	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
70	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
71	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
72	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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73	Phonon vibrational frequencies and elastic properties of solid SrFCl. An ab initio study. European Physical Journal B, 2005, 43, 453-461.	1.5	26
74	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
75	Serpentine polymorphism: a quantitative insight from first-principles calculations. CrystEngComm, 2016, 18, 4412-4419.	2.6	24
76	Infrared Investigation of Fluoride Occluded in Double Four-Member Rings in Zeolites. Journal of Physical Chemistry B, 2002, 106, 2796-2800.	2.6	23
77	Periodic density functional theory calculations for 3-dimensional polyacetylene with empirical dispersion terms. Physical Chemistry Chemical Physics, 2010, 12, 3289.	2.8	23
78	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
79	Periodic ab initio study of the oxidizing sites in Ti-containing zeolites. Journal of Molecular Catalysis A, 1997, 119, 449-458.	4.8	20
80	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
81	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
82	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
83	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
84	Ab initio quantumâ€mechanical simulation of the Raman spectrum of grossular. Journal of Raman Spectroscopy, 2009, 40, 416-418.	2.5	19
85	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
86	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
87	A periodic Hartreeâ€“Fock study of Na adsorption on the TiO2(110) rutile surface. Chemical Physics Letters, 1999, 303, 111-116.	2.6	18
88	Periodic ab initio study of silico-faujasite. Chemical Physics Letters, 1997, 277, 227-233.	2.6	16
89	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
90	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

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91	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
92	Hirshfeld-I charges in linear combination of atomic orbitals periodic calculations. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	16
93	The A-center defect in diamond: quantum mechanical characterization through the infrared spectrum. Physical Chemistry Chemical Physics, 2017, 19, 14478-14485.	2.8	16
94	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
95	Synthesis of Aluminosilicate Natrolites and Control of Their Tetrahedral Atom Ordering. Chemistry of Materials, 2014, 26, 3361-3363.	6.7	15
96	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
97	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
98	Periodic Hartree-Fock and density functional theory calculations for Li-doped polyacetylene chains. Journal of Chemical Physics, 2006, 124, 244703.	3.0	14
99	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
100	Orbital-controlled reactions catalysed by zeolites: Electrophilic alkylation of aromatics. Journal of Physical Organic Chemistry, 1994, 7, 364-370.	1.9	13
101	Comment on â€œAccurate Hartree-Fock energy of extended systems using large Gaussian basis setsâ€. Physical Review B, 2010, 81, .	3.2	13
102	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
103	Ab-initioquantum mechanical study of akdalaite (5Al₂O₃Â·) Tj ETQq1 1 0.784314 rgBT /Overlock 10 TF 012013.	0.4	12
104	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
105	Periodic Quantum Chemical Studies on Anhydrous and Hydrated Acid Clinoptilolite. Journal of Physical Chemistry A, 2014, 118, 5779-5789.	2.5	11
106	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
107	The Isobutyleneâ^'Isobutane Alkylation Process in Liquid HF Revisited. Journal of Physical Chemistry B, 2005, 109, 12946-12955.	2.6	10
108	The electronic structure of MgO nanotubes. An ab initio quantum mechanical investigation. Physical Chemistry Chemical Physics, 2013, 15, 13296.	2.8	10

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109	Charge distribution in NaY zeolite from charge-transfer molecular dynamics. Chemical Physics Letters, 2000, 327, 224-229.	2.6	9
110	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
111	On the use of symmetry in SCF calculations. The case of fullerenes and nanotubes. AIP Conference Proceedings, 2012, , .	0.4	9
112	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
113	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
114	Semiempirical Hamiltonians for spatially confined ?-electron systems. , 1996, 60, 971-981.		8
115	Ab-initio thermal physics and Cr-isotopic fractionation of MgCr2O4. American Mineralogist, 2007, 92, 98-108.	1.9	8
116	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
117	Ab initio modeling of layered materials with the CRYSTAL code: an overview. Zeitschrift FÃ¼r Kristallographie, 2009, 224, 241-250.	1.1	8
118	A fundamental connection between symmetry and spatial localization properties of basis sets. Theoretical Chemistry Accounts, 2010, 126, 165-175.	1.4	8
119	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
120	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
121	The constrained space orbital variation analysis for periodic ab initio calculations. Journal of Chemical Physics, 2006, 124, 194105.	3.0	7
122	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
123	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
124	Electronic structure characterization of six semiconductors through their localized Wannier functions. Physical Chemistry Chemical Physics, 2003, 5, 5319.	2.8	6
125	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
126	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

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127	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
128	Two points of view to look at symmetry. Journal of Physics: Conference Series, 2008, 117, 012030.	0.4	4
129	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
130	Beyond Wigner's theorems: The role of symmetry equivalences in quantum systems. International Journal of Quantum Chemistry, 2012, 112, 3543-3551.	2.0	3
131	Long-range exchange limit and dispersion in pure silica zeolites. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	3
132	Vibration Frequencies of Mg3Al2Si3O12 Pyrope. An ab initio Study with the CRYSTAL Code.. ChemInform, 2005, 36, no.	0.0	2
133	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
134	Coupled perturbed HF/KS calculation of the dielectric constant of crystalline systems. The case of six members of the garnet family. , 2012, , .		1
135	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
136	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
137	Can Cu+-Exchanged Zeolites Store Molecular Hydrogen? An ab initio Periodic Study Compared with Low-Temperature FTIR.. ChemInform, 2004, 35, no.	0.0	0