Lorenzo Maschio

List of Publications by Year
in descending order

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215 papers	11,561 citations	43973 48 h-index	32761 100 g-index
221 all docs	221 docs citations	221 times ranked	8310 citing authors

#	Article	IF	Citations
1	Quantumâ€mechanical condensed matter simulations with CRYSTAL. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1360.	6.2	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.	1.0	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, .	0.4	824
4	The calculation of static polarizabilities of 1â€3D periodic compounds. the implementation in the crystal code. Journal of Computational Chemistry, 2008, 29, 1450-1459.	1.5	253
5	Periodic local MP2 method for the study of electronic correlation in crystals: Theory and preliminary applications. Journal of Computational Chemistry, 2008, 29, 2113-2124.	1.5	216
6	Calculation of first and second static hyperpolarizabilities of one- to three-dimensional periodic compounds. Implementation in the <scp>CRYSTAL</scp> code.. Journal of Chemical Physics, 2008, 129, 244110.	1.2	199
7	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.	1.2	191
8	Ab-initio prediction of materials properties with CRYSTAL: MOF-5 as a case study. CrystEngComm, 2006, 8, 364-371.	1.3	187
9	Coupled perturbed Hartree-Fock for periodic systems: The role of symmetry and related computational aspects. Journal of Chemical Physics, 2008, 128, 014110.	1.2	186
10	Local-MP2 electron correlation method for nonconducting crystals. Journal of Chemical Physics, 2005, 122, 094113.	1.2	182
11	Effect of Benzoic Acid as a Modulator in the Structure of UiO-66: An Experimental and Computational Study. Journal of Physical Chemistry C, 2017, 121, 9312-9324.	1.5	176
12	Intermolecular Interaction Energies in Molecular Crystals: Comparison and Agreement of Localized MÃ¸llerâ€“Plesset 2, Dispersion-Corrected Density Functional, and Classical Empirical Two-Body Calculations. Journal of Physical Chemistry A, 2011, 115, 11179-11186.	1.1	169
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.	1.4	168
14	Ab initio analytical Raman intensities for periodic systems through a coupled perturbed Hartree-Fock/Kohn-Sham method in an atomic orbital basis. I. Theory. Journal of Chemical Physics, 2013, 139, 164101.	1.2	167
15	Spontaneous polarization as a Berry phase of the Hartree-Fock wave function: The case ofKNbO3. Physical Review B, 1997, 56, 10105-10114.	1.1	151
16	Ab initio analytical Raman intensities for periodic systems through a coupled perturbed Hartree-Fock/Kohn-Sham method in an atomic orbital basis. II. Validation and comparison with experiments. Journal of Chemical Physics, 2013, 139, 164102.	1.2	145
17	Vibrational spectrum of brucite, Mg(OH)2: a periodic ab initio quantum mechanical calculation including OH anharmonicity. Chemical Physics Letters, 2004, 396, 308-315.	1.2	142
18	Vibration Frequencies of Mg3Al2Si3O12 Pyrope. An ab Initio Study with the CRYSTAL Code. Journal of Physical Chemistry B, 2005, 109, 6146-6152.	1.2	142

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19	Fast local-MP2 method with density-fitting for crystals. I. Theory and algorithms. Physical Review B, 2007, 76, .	1.1	142
20	Ab initio analytical infrared intensities for periodic systems through a coupled perturbed Hartree-Fock/Kohn-Sham method. Journal of Chemical Physics, 2012, 137, 204113.	1.2	133
21	The CRYSTAL code, 1976â€“2020 and beyond, a long story. Journal of Chemical Physics, 2020, 152, 204111.	1.2	133
22	The Raman spectrum of CaCO3 polymorphs calcite and aragonite: A combined experimental and computational study. Journal of Chemical Physics, 2014, 140, 164509.	1.2	131
23	Cryscor: a program for the post-Hartreeâ€“Fock treatment of periodic systems. Physical Chemistry Chemical Physics, 2012, 14, 7615.	1.3	122
24	On the performance of eleven DFT functionals in the description of the vibrational properties of aluminosilicates. International Journal of Quantum Chemistry, 2010, 110, 406-415.	1.0	121
25	Ab Initio Quantum Simulation in Solid State Chemistry. Reviews in Computational Chemistry, 2005, , 1-125.	1.5	120
26	Performance of six functionals (LDA, PBE, PBESOL, B3LYP, PBE0, and WC1LYP) in the simulation of vibrational and dielectric properties of crystalline compounds. The case of forsterite Mg₂SiO₄. Journal of Computational Chemistry, 2011, 32, 1775-1784.	1.5	112
27	Elastic properties of six silicate garnet end members from accurate ab initio simulations. Physics and Chemistry of Minerals, 2014, 41, 151-160.	0.3	100
28	Fast local-MP2 method with density-fitting for crystals. II. Test calculations and application to the carbon dioxide crystal. Physical Review B, 2007, 76, .	1.1	92
29	The vibrational spectrum of CaCO3 aragonite: A combined experimental and quantum-mechanical investigation. Journal of Chemical Physics, 2013, 138, 014201.	1.2	92
30	Characterization of the electronic structure of crystalline compounds through their localized Wannier functions. Journal of Chemical Physics, 2002, 116, 1120-1127.	1.2	87
31	Assessment of Different Quantum Mechanical Methods for the Prediction of Structure and Cohesive Energy of Molecular Crystals. Journal of Chemical Theory and Computation, 2016, 12, 3340-3352.	2.3	85
32	The Multiple Structures of Vaterite. Crystal Growth and Design, 2013, 13, 2247-2251.	1.4	82
33	Periodic local MÃ¸llerâ€“Plesset second order perturbation theory method applied to molecular crystals: Study of solid NH3 and CO2 using extended basis sets. Journal of Chemical Physics, 2010, 132, 134706.	1.2	81
34	A new structural model for disorder in vaterite from first-principles calculations. CrystEngComm, 2012, 14, 44-47.	1.3	71
35	Structural, electronic and magnetic properties of KMF3(M=Mn, Fe, Co, Ni). Faraday Discussions, 1997, 106, 173-187.	1.6	64
36	Toward an Accurate Estimate of the Exfoliation Energy of Black Phosphorus: A Periodic Quantum Chemical Approach. Journal of Physical Chemistry Letters, 2016, 7, 131-136.	2.1	62

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37	Accurate dynamical structure factors from ab initio lattice dynamics: The case of crystalline silicon. Journal of Computational Chemistry, 2013, 34, 346-354.	1.5	61
38	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.	1.3	60
39	First-principles study of the mechanisms of the pressure-induced dielectric anomalies in ferroelectric perovskites. Phase Transitions, 2013, 86, 1069-1084.	0.6	57
40	Fitting of local densities in periodic systems. Physical Review B, 2008, 78, .	1.1	56
41	Local MP2 with Density Fitting for Periodic Systems: A Parallel Implementation. Journal of Chemical Theory and Computation, 2011, 7, 2818-2830.	2.3	55
42	Implementation of the finite field perturbation method in the CRYSTAL program for calculating the dielectric constant of periodic systems. Journal of Computational Chemistry, 2003, 24, 1305-1312.	1.5	52
43	Second Order Local MÃ‚ller-Plesset Perturbation Theory for Periodic Systems: the CRYSCOR Code. Zeitschrift Fur Physikalische Chemie, 2010, 224, 441-454.	1.4	52
44	High-pressure thermo-elastic properties of beryl (Al4Be6Si12O36) from ab initio calculations, and observations about the source of thermal expansion. Physics and Chemistry of Minerals, 2011, 38, 223-239.	0.3	52
45	Large-Scale B3LYP Simulations of Ibuprofen Adsorbed in MCM-41 Mesoporous Silica as Drug Delivery System. Journal of Physical Chemistry C, 2014, 118, 26737-26749.	1.5	52
46	First-principles optical response of semiconductors and oxide materials. Physical Review B, 2011, 83, .	1.1	51
47	Assessing thermochemical properties of materials through ab initio quantum-mechanical methods: the case of Î±-Al₂O₃. Physical Chemistry Chemical Physics, 2015, 17, 11670-11677.	1.3	51
48	Thermoelectric Properties of p-Type Cu₂O, CuO, and NiO from Hybrid Density Functional Theory. Journal of Physical Chemistry C, 2018, 122, 15180-15189.	1.5	51
49	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.	1.5	50
50	Thermodynamics and phonon dispersion of pyrope and grossular silicate garnets from ab initio simulations. Physics and Chemistry of Minerals, 2016, 43, 137-149.	0.3	50
51	Ab initio study of van der Waals and hydrogen-bonded molecular crystals with a periodic local-MP2 method. CrystEngComm, 2010, 12, 2429.	1.3	49
52	Approaching the theoretical limit in periodic local MP2 calculations with atomic-orbital basis sets: The case of LiH. Journal of Chemical Physics, 2011, 134, 214105.	1.2	49
53	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.	1.5	48
54	On the role of symmetry in the ab initio hartree-fock linear-combination-of-atomic-orbitals treatment of periodic systems. International Journal of Quantum Chemistry, 1986, 29, 1755-1774.	1.0	47

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55	Structure and stability of aluminium trihydroxides bayerite and gibbsite: A quantum mechanical ab initio study with the Crystal06 code. Chemical Physics Letters, 2008, 465, 220-225.	1.2	46
56	Regular chemisorption of hydrogen on graphite in the crystalline orbital NDO approximation. Journal of Chemical Physics, 1976, 65, 3075-3084.	1.2	43
57	The calculation of the static first and second susceptibilities of crystalline urea: A comparison of Hartreeâ€“Fock and density functional theory results obtained with the periodic coupled perturbed Hartreeâ€“Fock/Kohnâ€“Sham scheme. Journal of Chemical Physics, 2009, 131, 214704.	1.2	43
58	MP2 versus density-functional theory study of the Compton profiles of crystalline urea. Physical Review B, 2010, 81, .	1.1	43
59	A new massively parallel version of CRYSTAL for large systems on high performance computing architectures. Journal of Computational Chemistry, 2012, 33, 2276-2284.	1.5	43
60	Periodic local MP2 method employing orbital specific virtuals. Journal of Chemical Physics, 2015, 143, 102805.	1.2	43
61	Performance of 12 DFT functionals in the study of crystal systems: Al₂SiO₅ orthosilicates and Al hydroxides as a case study. International Journal of Quantum Chemistry, 2010, 110, 2260-2273.	1.0	42
62	Substitutional nitrogen in diamond: A quantum mechanical investigation of the electronic and spectroscopic properties. Carbon, 2018, 134, 354-365.	5.4	42
63	The vibrational spectrum of lizardite-1T [Mg3Si2O5(OH)4] at the Â point: A contribution from an ab initio periodic B3LYP calculation. American Mineralogist, 2009, 94, 986-994.	0.9	41
64	Structure and energetics of imogolite: a quantum mechanical ab initio study with B3LYP hybrid functional. Journal of Materials Chemistry, 2010, 20, 10417.	6.7	41
65	Raman spectrum of NaAlSi₂O₆ jadeite. A quantum mechanical simulation. Journal of Raman Spectroscopy, 2014, 45, 703-709.	1.2	41
66	Periodic density functional theory and local-MP2 study of the librational modes of Ice XI. Journal of Chemical Physics, 2009, 130, 074505.	1.2	39
67	On choosing the best density functional approximation. Chemical Modelling, 0, , 168-185.	0.2	38
68	Anharmonic Vibrational States of Solids from DFT Calculations. Part II: Implementation of the VSCF and VCI Methods. Journal of Chemical Theory and Computation, 2019, 15, 3766-3777.	2.3	37
69	Periodic approach to the electronic structure and magnetic coupling in KCuF3, K2CuF4, and Sr2CuO2Cl2 low-dimensional magnetic systems. International Journal of Quantum Chemistry, 2004, 99, 805-823.	1.0	36
70	DFT and Local-MP2 Periodic Study of the Structure and Stability of Two Proton-Ordered Polymorphs of Ice. Journal of Physical Chemistry B, 2009, 113, 2347-2354.	1.2	36
71	Examining the Accuracy of Density Functional Theory for Predicting the Thermodynamics of Water Incorporation into Minerals: The Hydrates of Calcium Carbonate. Journal of Physical Chemistry C, 2013, 117, 17814-17823.	1.5	36
72	Periodic and fragment models based on the local correlation approach. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1357.	6.2	36

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73	Anharmonic Vibrational States of Solids from DFT Calculations. Part I: Description of the Potential Energy Surface. Journal of Chemical Theory and Computation, 2019, 15, 3755-3765.	2.3	36
74	Exfoliation Energy of Layered Materials by DFT-D: Beware of Dispersion!. Journal of Chemical Theory and Computation, 2020, 16, 5244-5252.	2.3	35
75	Periodic quantum mechanical simulation of the Heâ€“MgO(100) interaction potential. Journal of Chemical Physics, 2011, 134, 014706.	1.2	34
76	On the use of symmetry in configurational analysis for the simulation of disordered solids. Journal of Physics Condensed Matter, 2013, 25, 105401.	0.7	34
77	Ab Initio Periodic Simulation of the Spectroscopic and Optical Properties of Novel Porous Graphene Phases. Journal of Physical Chemistry C, 2013, 117, 2222-2229.	1.5	33
78	Exfoliation Energy of Black Phosphorus Revisited: A Coupled Cluster Benchmark. Journal of Physical Chemistry Letters, 2017, 8, 1290-1294.	2.1	33
79	Pressure-induced transitions in solid nitrogen: Role of dispersive interactions. Physical Review B, 2011, 84, .	1.1	32
80	Ab initio electronic transport and thermoelectric properties of solids from full and range-separated hybrid functionals. Journal of Chemical Physics, 2017, 147, 114101.	1.2	32
81	The First and Second Static Electronic Hyperpolarizabilities of Zigzag Boron Nitride Nanotubes. An ab Initio Approach through the Coupled Perturbed Kohnâ€“Sham Scheme. Journal of Physical Chemistry A, 2011, 115, 12631-12637.	1.1	31
82	Geometrical frustration of an argon monolayer adsorbed on the MgO (100) surface: An accurate periodicab initiostudy. Physical Review B, 2012, 86, .	1.1	31
83	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.	1.3	31
84	Computation of Second Harmonic Generation for Crystalline Urea and KDP. An ab Initio Approach through the Coupled Perturbed Hartreeâ€“Fock/Kohnâ€“Sham Scheme. Journal of Chemical Theory and Computation, 2016, 12, 107-113.	2.3	31
85	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.	1.3	30
86	Beyond a Hartreeâ€“Fock description of crystalline solids: the case of lithium hydride. Theoretical Chemistry Accounts, 2007, 117, 781-791.	0.5	29
87	The IR vibrational properties of six members of the garnet family: A quantum mechanical ab initio study. American Mineralogist, 2011, 96, 1787-1798.	0.9	28
88	Comment on â€œAb initio analytical infrared intensities for periodic systems through a coupled perturbed Hartree-Fock/Kohn-Sham methodâ€•[J. Chem. Phys. 137, 204113 (2012)]. Journal of Chemical Physics, 2013, 139, 167101.	1.2	28
89	Raman spectroscopic features of the neutral vacancy in diamond from ab initio quantum-mechanical calculations. Physical Chemistry Chemical Physics, 2016, 18, 1961-1968.	1.3	27
90	Single-layered chrysotile nanotubes: A quantum mechanical ab initio simulation. Journal of Chemical Physics, 2009, 131, 204701.	1.2	26

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91	Beyond a single-determinantal description of the density matrix of periodic systems: Experimental versus theoretical Compton profiles of crystalline silicon. Physical Review B, 2011, 83, .	1.1	26
92	The electronic states of the neutral vacancy in diamond: a quantum mechanical approach. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	26
93	Electron correlation decides the stability of cubic versus hexagonal boron nitride. Physical Review B, 2011, 83, .	1.1	25
94	Raman Spectrum of Pyrope Garnet. A Quantum Mechanical Simulation of Frequencies, Intensities, and Isotope Shifts. Journal of Physical Chemistry A, 2013, 117, 11464-11471.	1.1	25
95	Quantum-mechanical calculation of the vibrational spectrum of beryl (Al4Be6Si12O36) at the Î“ point. Physics and Chemistry of Minerals, 2006, 33, 519-532.	0.3	24
96	Calculation of the dielectric constant Ïµ and first nonlinear susceptibility Ï‡(2) of crystalline potassium dihydrogen phosphate by the coupled perturbed Hartreeâ€“Fock and coupled perturbed Kohnâ€“Sham schemes as implemented in the <scp>CRYSTAL</scp> code. Journal of Chemical Physics, 2009, 131, 204509.	1.2	24
97	Evidence of instantaneous electron correlation from Compton profiles of crystalline silicon. Physical Chemistry Chemical Physics, 2011, 13, 933-936.	1.3	24
98	A post-Hartreeâ€“Fock study of pressure-induced phase transitions in solid nitrogen: The case of the Î±, Î³, and Îµ low-pressure phases. Journal of Chemical Physics, 2011, 134, 074502.	1.2	24
99	Symmetry and random sampling of symmetry independent configurations for the simulation of disordered solids. Journal of Physics Condensed Matter, 2013, 25, 355401.	0.7	24
100	Double-hybrid density-functional theory applied to molecular crystals. Journal of Chemical Physics, 2014, 141, 044105.	1.2	24
101	Benchmarking dispersion and geometrical counterpoise corrections for costâ€effective largeâ€scale DFT calculations of water adsorption on graphene. Journal of Computational Chemistry, 2014, 35, 1789-1800.	1.5	24
102	Dual luminescence in solid CuI(piperazine): hypothesis of an emissive 1-D delocalized excited state. Dalton Transactions, 2015, 44, 13003-13006.	1.6	24
103	Exploring the Linear Optical Properties of Borazine (B₃N₃) Doped Graphenes. 0D Flakes vs 2D Sheets. Journal of Physical Chemistry C, 2017, 121, 709-722.	1.5	24
104	Calculation of the Infrared Intensity of Crystalline Systems. A Comparison of Three Strategies Based on Berry Phase, Wannier Function, and Coupled-Perturbed Kohnâ€“Sham Methods. Journal of Physical Chemistry C, 2019, 123, 8336-8346.	1.5	24
105	Local MP2 periodic study of rare-gas crystals. Chemical Physics Letters, 2009, 467, 294-298.	1.2	23
106	Polarizability and hyperpolarizability of BN zigzag nanotubes calculated by the coupled perturbed Kohn-Sham scheme. Physical Review B, 2011, 83, .	1.1	23
107	Oxalyl dihydrazide polymorphism: a periodic dispersion-corrected DFT and MP2 investigation. CrystEngComm, 2014, 16, 102-109.	1.3	23
108	Characterization of the B-Center Defect in Diamond through the Vibrational Spectrum: A Quantum-Mechanical Approach. Journal of Physical Chemistry A, 2018, 122, 594-600.	1.1	23

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109	Periodic ab initio estimates of the dispersive interaction between molecular nitrogen and a monolayer of hexagonal BN. Physical Chemistry Chemical Physics, 2011, 13, 4434.	1.3	22
110	The infrared spectrum of ortho-enstatite from reflectance experiments and first-principle simulations. Monthly Notices of the Royal Astronomical Society, 2012, 420, 147-154.	1.6	22
111	Calculation of longitudinal polarizability and second hyperpolarizability of polyacetylene with the coupled perturbed Hartree-Fock/Kohn-Sham scheme: Where it is shown how finite oligomer chains tend to the infinite periodic polymer. Journal of Chemical Physics, 2012, 136, 114101.	1.2	21
112	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.	1.2	21
113	Range-separated double-hybrid density-functional theory applied to periodic systems. Journal of Chemical Physics, 2015, 143, 102811.	1.2	21
114	Elucidating the fundamental forces in protein crystal formation: the case of crambin. Chemical Science, 2016, 7, 1496-1507.	3.7	21
115	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.	1.0	20
116	The VN₃H defect in diamond: a quantum-mechanical characterization. Physical Chemistry Chemical Physics, 2017, 19, 22221-22229.	1.3	20
117	The characterization of the VN H defects in diamond through the infrared vibrational spectrum. A quantum mechanical investigation. Carbon, 2018, 132, 210-219.	5.4	20
118	Quantum-mechanical ab initio simulation of the Raman and IR spectra of Mn3Al2Si3O12 spessartine. Physics and Chemistry of Minerals, 2009, 36, 415-420.	0.3	19
119	Search and Characterization of Transition State Structures in Crystalline Systems Using Valence Coordinates. Journal of Chemical Theory and Computation, 2010, 6, 1341-1350.	2.3	19
120	The infrared spectrum of spessartine <mml:math altimg="si69.gif" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="http://www.elsevie.	1.2	19
121	Calculation of the dynamic first electronic hyperpolarizability Î²(â^'Ï‰ Ïƒ; Ï‰1,) Tj ETQq1 1 0.784314 rgB Chemical Physics, 2015, 143, 244102.	1.2	19
122	Fragment-Based Direct-Local-Ring-Coupled-Cluster Doubles Treatment Embedded in the Periodic Hartreeâ€“Fock Solution. Journal of Chemical Theory and Computation, 2016, 12, 5145-5156.	2.3	19
123	Nitrogen substitutional defects in silicon. A quantum mechanical investigation of the structural, electronic and vibrational properties. Physical Chemistry Chemical Physics, 2019, 21, 20939-20950.	1.3	19
124	Calculation of the static electronic second hyperpolarizability or Ï‡(3) tensor of three-dimensional periodic compounds with a local basis set. Journal of Chemical Physics, 2009, 131, 184105.	1.2	18
125	Oneâ€Dimensional Phosphorus Nanostructures: from Nanorings to Nanohelices. Chemistry - A European Journal, 2017, 23, 15884-15888.	1.7	18
126	Gaussian Basis Sets for Crystalline Solids: All-Purpose Basis Set Libraries vs System-Specific Optimizations. Journal of Chemical Theory and Computation, 2020, 16, 2192-2201.	2.3	18

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127	Approaching an exact treatment of electronic correlations at solid surfaces: The binding energy of the lowest bound state of helium adsorbed on MgO(100). Physical Review B, 2014, 89, .	1.1	17
128	Vibrational spectroscopy of hydrogens in diamond: a quantum mechanical treatment. Physical Chemistry Chemical Physics, 2018, 20, 11930-11940.	1.3	17
129	Direct inversion of the iterative subspace (DIIS) convergence accelerator for crystalline solids employing Gaussian basis sets. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	17
130	The VN2 negatively charged defect in diamond. A quantum mechanical investigation of the EPR response. Carbon, 2020, 159, 443-450.	5.4	17
131	Periodic local-MP2 computational study of crystalline neon. Physical Chemistry Chemical Physics, 2009, 11, 586-592.	1.3	16
132	Vibrational contribution to static and dynamic (Hyper)polarizabilities of zigzag BN nanotubes calculated by the finite field nuclear relaxation method. International Journal of Quantum Chemistry, 2012, 112, 2160-2170.	1.0	16
133	Elasticity of grossularâ€“andradite solid solution: an ab initio investigation. Physical Chemistry Chemical Physics, 2014, 16, 15331.	1.3	16
134	The A-center defect in diamond: quantum mechanical characterization through the infrared spectrum. Physical Chemistry Chemical Physics, 2017, 19, 14478-14485.	1.3	16
135	Nuclearâ€relaxed elastic and piezoelectric constants of materials: Computational aspects of two quantumâ€mechanical approaches. Journal of Computational Chemistry, 2017, 38, 257-264.	1.5	16
136	Low energy excitations in NiO based on a direct Î”-SCF approach. Journal of Physics Condensed Matter, 2018, 30, 495901.	0.7	16
137	Hydrogen, boron and nitrogen atoms in diamond: a quantum mechanical vibrational analysis. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	16
138	Key Role of Defects in Thermoelectric Performance of TiMSn (M = Ni, Pd, and Pt) Half-Heusler Alloys. Journal of Physical Chemistry C, 2020, 124, 14997-15006.	1.5	16
139	Regular chemisorption of hydrogen on graphite in the COâ€“NDO approximation. II. Journal of Chemical Physics, 1976, 65, 4116-4120.	1.2	15
140	A local MP2 periodic study of crystalline argon. Journal of Physics: Conference Series, 2008, 117, 012007.	0.3	15
141	Third-Order Electric Field Response of Infinite Linear Chains Composed of Phenalenyl Radicals. Journal of Physical Chemistry C, 2016, 120, 6756-6761.	1.5	15
142	On the exfoliation and anisotropic thermal expansion of black phosphorus. Chemical Communications, 2018, 54, 9793-9796.	2.2	15
143	Local ab initio methods for calculating optical bandgaps in periodic systems. II. Periodic density fitted local configuration interaction singles method for solids. Journal of Chemical Physics, 2012, 137, 204119.	1.2	14
144	Intermolecular modulation of IR intensities in the solid state. The role of weak interactions in polyethylene crystal: A computational DFT study. Journal of Chemical Physics, 2016, 145, 144901.	1.2	14

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145	A local-MP2 approach to the ab initio study of electron correlation in crystals and to the simulation of vibrational spectra: the case of Ice XI. Theoretical Chemistry Accounts, 2009, 123, 327-335.	0.5	13
146	Comment on â€œAccurate Hartree-Fock energy of extended systems using large Gaussian basis setsâ€• Physical Review B, 2010, 81, .	1.1	13
147	The infrared vibrational spectrum of andradite-grossular solid solutions: A quantum mechanical simulation. American Mineralogist, 2013, 98, 966-976.	0.9	13
148	Comparison between cluster and supercell approaches: the case of defects in diamond. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	13
149	Salicylideneaniline-Based Covalent Organic Frameworks: A New Family of Multistate Second-Order Nonlinear Optical Switches. Journal of Physical Chemistry C, 2020, 124, 24451-24459.	1.5	13
150	On the Prospective Use of the One-Electron Density Matrix as a Test of the Quality of Post-Hartreeâ€“Fock Schemes for Crystals. Zeitschrift Fur Physikalische Chemie, 2006, 220, 913-926.	1.4	12
151	Use of ab initio methods for the interpretation of the experimental IR reflectance spectra of crystalline compounds. Journal of Computational Chemistry, 2013, 34, 1476-1485.	1.5	12
152	Dispersion corrected DFT calculations for the adsorption of N2O on MgO. Surface Science, 2014, 627, 11-15.	0.8	12
153	Electron Correlation at the MgF₂(110) Surface: A Comparison of Incremental and Local Correlation Methods. Journal of Chemical Theory and Computation, 2015, 11, 252-259.	2.3	12
154	Ab initio periodic study of the conformational behavior of glycine helical homopeptides. Journal of Computational Chemistry, 2010, 31, 1777-1784.	1.5	11
155	He-atom scattering from MgO(100): calculating diffraction peak intensities with a semi ab initio potential. Physical Chemistry Chemical Physics, 2011, 13, 14750.	1.3	11
156	Diffraction of helium on MgO(100) surface calculated from first-principles. Physical Chemistry Chemical Physics, 2014, 16, 21106-21113.	1.3	11
157	Direct Piezoelectric Tensor of 3D Periodic Systems through a Coupled Perturbed Hartreeâ€“Fock/Kohnâ€“Sham Method. Zeitschrift Fur Physikalische Chemie, 2016, 230, 719-736.	1.4	11
158	Folic Acid in the Solid State: A Synergistic Computational, Spectroscopic, and Structural Approach. Crystal Growth and Design, 2016, 16, 2218-2224.	1.4	11
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