Lorenzo Maschio

List of Publications by Year
in descending order

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215 papers	11,561 citations	44069 48 h-index	32842 100 g-index
221 all docs	221 docs citations	221 times ranked	8310 citing authors

#	Article	IF	Citations
1	The superexchange mechanism in crystalline compounds. The case of KMF₃ (M = Mn, Fe, Co,) Tj ETQq1 1 0.784314 rgBT	1.8	3
2	Reaction barriers on non-conducting surfaces beyond periodic local MP2: Diffusion of hydrogen on Î±-Al2O3(0001) as a test case. Journal of Chemical Physics, 2022, 156, 074109.	3.0	5
3	Electrical control of orbital and vibrational interlayer coupling in bi- and trilayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>2</mml:mn><mml:mi mathvariant="normal">H</mml:mi><mml:mtext>â^'</mml:mtext><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:mrow></mml:math> Physical Review Materials, 2022, 6, .	2.4	4
4	Raman activity of the longitudinal optical phonons of the LiNbO₃ crystal: Experimental determination and quantum mechanical simulation. Journal of Raman Spectroscopy, 2022, 53, 1904-1914.	2.5	3
5	Electronic Excitations in Crystalline Solids through the Maximum Overlap Method. Journal of Chemical Theory and Computation, 2021, 17, 6073-6079.	5.3	4
6	Doping the permanent magnet CeFe11Ti with Co and Ni using ab-initio density functional methods. Physica B: Condensed Matter, 2021, 620, 413241.	2.7	3
7	The NVâ^'â¯N+ charged pair in diamond: a quantum-mechanical investigation. Physical Chemistry Chemical Physics, 2021, 23, 18724-18733.	2.8	2
8	The VN2 negatively charged defect in diamond. A quantum mechanical investigation of the EPR response. Carbon, 2020, 159, 443-450.	10.3	17
9	Coupled Perturbation Theory Approach to Dual Basis Sets for Molecules and Solids. 1. General Theory and Application to Molecules. Journal of Chemical Theory and Computation, 2020, 16, 340-353.	5.3	7
10	Ab initio compressibility of metastable low albite: revealing a lambda-type singularity at pressures of the Earthâ€™s upper mantle. Physics and Chemistry of Minerals, 2020, 47, 1.	0.8	3
11	Salicylideneaniline-Based Covalent Organic Frameworks: A New Family of Multistate Second-Order Nonlinear Optical Switches. Journal of Physical Chemistry C, 2020, 124, 24451-24459.	3.1	13
12	Representation of the virtual space in extended systems â€“ a correlation energy convergence study. Molecular Physics, 2020, 118, e1733118.	1.7	10
13	Fragment-Based Restricted Active Space Configuration Interaction with Second-Order Corrections Embedded in Periodic Hartreeâ€“Fock Wave Function. Journal of Chemical Theory and Computation, 2020, 16, 7100-7108.	5.3	11
14	From anisotropy of dielectric tensors to birefringence: a quantum mechanics approach. Rendiconti Lincei, 2020, 31, 835-851.	2.2	3
15	Interstitial defects in diamond: A quantum mechanical simulation of their EPR constants and vibrational spectra. Journal of Chemical Physics, 2020, 153, 024119.	3.0	6
16	Predicted strong spin-phonon interactions in Li-doped diamond. Physical Chemistry Chemical Physics, 2020, 22, 20612-20617.	2.8	5
17	First principles calculations of the vibrational properties of single and dimer F-type centers in corundum crystals. Journal of Chemical Physics, 2020, 153, 134107.	3.0	5
18	The CRYSTAL code, 1976â€“2020 and beyond, a long story. Journal of Chemical Physics, 2020, 152, 204111.	3.0	133

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19	N₂ positively charged defects in diamond. A quantum mechanical investigation of the structural, electronic, EPR and vibrational properties. Journal of Materials Chemistry C, 2020, 8, 5239-5247.	5.5	10
20	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.	5.3	18
21	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.	3.1	16
22	Exfoliation Energy of Layered Materials by DFT-D: Beware of Dispersion!. Journal of Chemical Theory and Computation, 2020, 16, 5244-5252.	5.3	35
23	The spectroscopic characterization of interstitial oxygen in bulk silicon: A quantum mechanical simulation. Journal of Chemical Physics, 2020, 152, 054502.	3.0	5
24	Hybrid-functional electronic structure of multilayer graphene. Physical Review B, 2020, 101, .	3.2	7
25	Substitutional carbon defects in silicon: A quantum mechanical characterization through the infrared and Raman spectra. Journal of Computational Chemistry, 2020, 41, 1638-1644.	3.3	8
26	Evolutionary Algorithmâ€Based Crystal Structure Prediction for Copper(I) Fluoride. Chemistry - A European Journal, 2019, 25, 11528-11537.	3.3	6
27	Nitrogen interstitial defects in silicon. A quantum mechanical investigation of the structural, electronic and vibrational properties. Materials Today Communications, 2019, 21, 100616.	1.9	9
28	Nitrogen substitutional defects in silicon. A quantum mechanical investigation of the structural, electronic and vibrational properties. Physical Chemistry Chemical Physics, 2019, 21, 20939-20950.	2.8	19
29	On the Models for the Investigation of Charged Defects in Solids: The Case of the VN^{â€“} Defect in Diamond. Journal of Physical Chemistry A, 2019, 123, 4806-4815.	2.5	4
30	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.	5.3	36
31	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.	5.3	37
32	Substitutional boron and nitrogen pairs in diamond. A quantum mechanical vibrational analysis. Carbon, 2019, 146, 709-716.	10.3	10
33	The CeFe₁₁Ti permanent magnet: a closer look at the microstructure of the compound. Journal of Physics Condensed Matter, 2019, 31, 505505.	1.8	6
34	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.	3.1	24
35	The characterization of the VN H defects in diamond through the infrared vibrational spectrum. A quantum mechanical investigation. Carbon, 2018, 132, 210-219.	10.3	20
36	Quantumâ€mechanical condensed matter simulations with CRYSTAL. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1360.	14.6	1,277

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37	Experimental and Theoretical Infrared Signatures of REMO₃ (RE = La, Pr, Nd, Sm, and M =) Tj ETQq1 1 0.784314 rgBT /Over	3.1	8
38	Vibrational spectroscopy of hydrogens in diamond: a quantum mechanical treatment. Physical Chemistry Chemical Physics, 2018, 20, 11930-11940.	2.8	17
39	Substitutional nitrogen in diamond: A quantum mechanical investigation of the electronic and spectroscopic properties. Carbon, 2018, 134, 354-365.	10.3	42
40	Looking for $$sp^2$$ s p 2 carbon atoms in diamond: a quantum mechanical study of interacting vacancies. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	8
41	Periodic and fragment models based on the local correlation approach. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1357.	14.6	36
42	Ab initio calculation of nonlinear optical properties for chiral carbon nanotubes. Second harmonic generation and dc-Pockels effect. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	4
43	Direct inversion of the iterative subspace (DIIS) convergence accelerator for crystalline solids employing Gaussian basis sets. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	17
44	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.	2.5	23
45	Scalars, vectors and tensors evolving from slabs to bulk. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	0
46	Low energy excitations in NiO based on a direct Î”-SCF approach. Journal of Physics Condensed Matter, 2018, 30, 495901.	1.8	16
47	Hydrogen, boron and nitrogen atoms in diamond: a quantum mechanical vibrational analysis. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	16
48	Implicit Solvation Using a Generalized Finite-Difference Approach in CRYSTAL: Implementation and Results for Molecules, Polymers, and Surfaces. Journal of Chemical Theory and Computation, 2018, 14, 5969-5983.	5.3	8
49	Interstitial nitrogen atoms in diamond. A quantum mechanical investigation of its electronic and vibrational properties. Physical Chemistry Chemical Physics, 2018, 20, 16615-16624.	2.8	10
50	On the exfoliation and anisotropic thermal expansion of black phosphorus. Chemical Communications, 2018, 54, 9793-9796.	4.1	15
51	Thermoelectric Properties of p-Type Cu₂O, CuO, and NiO from Hybrid Density Functional Theory. Journal of Physical Chemistry C, 2018, 122, 15180-15189.	3.1	51
52	Dispersion interactions in silicon allotropes. Physical Chemistry Chemical Physics, 2017, 19, 7699-7707.	2.8	7
53	Exfoliation Energy of Black Phosphorus Revisited: A Coupled Cluster Benchmark. Journal of Physical Chemistry Letters, 2017, 8, 1290-1294.	4.6	33
54	Comparison between cluster and supercell approaches: the case of defects in diamond. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	13

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55	Topical collection of papers collected on the occasion of the XLI congress of the theoretical chemists of Latin expression (CHITEL 2015 - Torino - Italy). Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	0
56	One Step Toward a New Generation of C-MOS Compatible Oxide Pâ€“N Junctions: Structure of the LSMO/ZnO Interface Elucidated by an Experimental and Theoretical Synergic Work. ACS Applied Materials & Interfaces, 2017, 9, 20974-20980.	8.0	4
57	The A-center defect in diamond: quantum mechanical characterization through the infrared spectrum. Physical Chemistry Chemical Physics, 2017, 19, 14478-14485.	2.8	16
58	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.	3.1	176
59	Exploring the Linear Optical Properties of Borazine (B₃N₃) Doped Graphenes. 0D Flakes vs 2D Sheets. Journal of Physical Chemistry C, 2017, 121, 709-722.	3.1	24
60	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
61	Ab Initio Simulation of ZnO/LaMnO₃ Heterojunctions: Insights into Their Structural and Electronic Properties. Journal of Physical Chemistry C, 2017, 121, 25333-25341.	3.1	2
62	Ab initio electronic transport and thermoelectric properties of solids from full and range-separated hybrid functionals. Journal of Chemical Physics, 2017, 147, 114101.	3.0	32
63	Oneâ€Dimensional Phosphorus Nanostructures: from Nanorings to Nanohelices. Chemistry - A European Journal, 2017, 23, 15884-15888.	3.3	18
64	The VN₃H defect in diamond: a quantum-mechanical characterization. Physical Chemistry Chemical Physics, 2017, 19, 22221-22229.	2.8	20
65	Electromechanical Properties of Ba_(1â€“x)Sr_xTiO₃ Perovskite Solid Solutions from First-Principles Calculations. Journal of Physical Chemistry A, 2017, 121, 9409-9414.	2.5	11
66	BiVO3 : A Bi-based material with promising uv-visible light absorption properties. Physical Review B, 2017, 96, .	3.2	11
67	On the Use of Benchmarks for Multiple Properties. Computation, 2016, 4, 20.	2.0	7
68	The unique Raman fingerprint of boron nitride substitution patterns in graphene. Physical Chemistry Chemical Physics, 2016, 18, 20270-20275.	2.8	9
69	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.	3.0	14
70	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.	5.3	19
71	Spin susceptibility and electron-phonon coupling of two-dimensional materials by range-separated hybrid density functionals: Case study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>Li</mml:mi></mml:mrow><mml:mi>x</mml:mi></mml:msub></mml:math> Physical Review B, 2016, 94, .	3.2	5
72	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

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73	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.	5.3	85
74	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
75	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.	4.6	62
76	Third-Order Electric Field Response of Infinite Linear Chains Composed of Phenalenyl Radicals. Journal of Physical Chemistry C, 2016, 120, 6756-6761.	3.1	15
77	Thermodynamics and phonon dispersion of pyrope and grossular silicate garnets from ab initio simulations. Physics and Chemistry of Minerals, 2016, 43, 137-149.	0.8	50
78	The electronic states of the neutral vacancy in diamond: a quantum mechanical approach. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	26
79	Folic Acid in the Solid State: A Synergistic Computational, Spectroscopic, and Structural Approach. Crystal Growth and Design, 2016, 16, 2218-2224.	3.0	11
80	Elucidating the fundamental forces in protein crystal formation: the case of crambin. Chemical Science, 2016, 7, 1496-1507.	7.4	21
81	Raman spectroscopic features of the neutral vacancy in diamond from ab initio quantum-mechanical calculations. Physical Chemistry Chemical Physics, 2016, 18, 1961-1968.	2.8	27
82	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.	5.3	31
83	Calculation of the dynamic first electronic hyperpolarizability Î²(â^'Ï‰ Ïƒ; Ï‰1,) Tj ETQq1 1 0.784314 rgB Chemical Physics, 2015, 143, 244102.	3.0	19
84	Range-separated double-hybrid density-functional theory applied to periodic systems. Journal of Chemical Physics, 2015, 143, 102811.	3.0	21
85	Quantum-mechanical simulation of the IR reflectance spectrum of Mn3Al2Si3O12 spessartine. , 2015, , .		0
86	Periodic local MP2 method employing orbital specific virtuals. Journal of Chemical Physics, 2015, 143, 102805.	3.0	43
87	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.	5.3	12
88	Dual luminescence in solid CuI(piperazine): hypothesis of an emissive 1-D delocalized excited state. Dalton Transactions, 2015, 44, 13003-13006.	3.3	24
89	Assessing thermochemical properties of materials through ab initio quantum-mechanical methods: the case of Î±-Al₂O₃. Physical Chemistry Chemical Physics, 2015, 17, 11670-11677.	2.8	51
90	The effect of electron correlation on the adsorption of hydrogen fluoride and water on magnesium fluoride surfaces. Physical Chemistry Chemical Physics, 2015, 17, 18722-18728.	2.8	9

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91	Double-hybrid density-functional theory applied to molecular crystals. Journal of Chemical Physics, 2014, 141, 044105.	3.0	24
92	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, .	3.2	17
93	The Raman spectrum of CaCO3 polymorphs calcite and aragonite: A combined experimental and computational study. Journal of Chemical Physics, 2014, 140, 164509.	3.0	131
94	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
95	Elastic properties of six silicate garnet end members from accurate ab initio simulations. Physics and Chemistry of Minerals, 2014, 41, 151-160.	0.8	100
96	Binding is responsible for exceptional hardness in polyethylene/silicalite nanocomposite materials. CrystEngComm, 2014, 16, 10177-10180.	2.6	0
97	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.	3.1	52
98	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
99	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
100	Diffraction of helium on MgO(100) surface calculated from first-principles. Physical Chemistry Chemical Physics, 2014, 16, 21106-21113.	2.8	11
101	Elasticity of grossularâ€“andradite solid solution: an ab initio investigation. Physical Chemistry Chemical Physics, 2014, 16, 15331.	2.8	16
102	Oxalyl dihydrazide polymorphism: a periodic dispersion-corrected DFT and MP2 investigation. CrystEngComm, 2014, 16, 102-109.	2.6	23
103	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
104	Raman spectrum of NaAlSi₂O₆ jadeite. A quantum mechanical simulation. Journal of Raman Spectroscopy, 2014, 45, 703-709.	2.5	41
105	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.	3.3	24
106	The Raman spectrum of grossular garnet: a quantum mechanical simulation of wavenumbers and intensities. Journal of Raman Spectroscopy, 2014, 45, 710-715.	2.5	10
107	Dispersion corrected DFT calculations for the adsorption of N2O on MgO. Surface Science, 2014, 627, 11-15.	1.9	12
108	On the use of symmetry in configurational analysis for the simulation of disordered solids. Journal of Physics Condensed Matter, 2013, 25, 105401.	1.8	34

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109	Symmetry and random sampling of symmetry independent configurations for the simulation of disordered solids. Journal of Physics Condensed Matter, 2013, 25, 355401.	1.8	24
110	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.	3.0	167
111	First-principles study of the mechanisms of the pressure-induced dielectric anomalies in ferroelectric perovskites. Phase Transitions, 2013, 86, 1069-1084.	1.3	57
112	Accurate dynamical structure factors from ab initio lattice dynamics: The case of crystalline silicon. Journal of Computational Chemistry, 2013, 34, 346-354.	3.3	61
113	Ab Initio Periodic Simulation of the Spectroscopic and Optical Properties of Novel Porous Graphene Phases. Journal of Physical Chemistry C, 2013, 117, 2222-2229.	3.1	33
114	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.	3.3	12
115	The Multiple Structures of Vaterite. Crystal Growth and Design, 2013, 13, 2247-2251.	3.0	82
116	The electronic structure of MgO nanotubes. An ab initio quantum mechanical investigation. Physical Chemistry Chemical Physics, 2013, 15, 13296.	2.8	10
117	The infrared vibrational spectrum of andradite-grossular solid solutions: A quantum mechanical simulation. American Mineralogist, 2013, 98, 966-976.	1.9	13
118	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.	3.1	36
119	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
120	The vibrational spectrum of CaCO3 aragonite: A combined experimental and quantum-mechanical investigation. Journal of Chemical Physics, 2013, 138, 014201.	3.0	92
121	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.	3.0	28
122	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.	3.0	145
123	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.	3.0	21
124	Nuclear motion effects on the density matrix of crystals: An ab initio Monte Carlo harmonic approach. Journal of Chemical Physics, 2012, 137, 044114.	3.0	7
125	Geometrical frustration of an argon monolayer adsorbed on the MgO (100) surface: An accurate periodicab initiostudy. Physical Review B, 2012, 86, .	3.2	31
126	Ab initio analytical infrared intensities for periodic systems through a coupled perturbed Hartree-Fock/Kohn-Sham method. Journal of Chemical Physics, 2012, 137, 204113.	3.0	133

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127	Cryscor: a program for the post-Hartreeâ€“Fock treatment of periodic systems. Physical Chemistry Chemical Physics, 2012, 14, 7615.	2.8	122
128	A new structural model for disorder in vaterite from first-principles calculations. CrystEngComm, 2012, 14, 44-47.	2.6	71
129	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.	3.0	14
130	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.	2.0	16
131	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
132	A new massively parallel version of CRYSTAL for large systems on high performance computing architectures. Journal of Computational Chemistry, 2012, 33, 2276-2284.	3.3	43
133	Structural Characteristics of Graphaneâ€Type C and BN Nanostructures by Periodic Local MP2 Approach. ChemPhysChem, 2012, 13, 2361-2367.	2.1	9
134	The infrared spectrum of ortho-enstatite from reflectance experiments and first-principle simulations. Monthly Notices of the Royal Astronomical Society, 2012, 420, 147-154.	4.4	22
135	Evidence of instantaneous electron correlation from Compton profiles of crystalline silicon. Physical Chemistry Chemical Physics, 2011, 13, 933-936.	2.8	24
136	Periodic ab initio estimates of the dispersive interaction between molecular nitrogen and a monolayer of hexagonal BN. Physical Chemistry Chemical Physics, 2011, 13, 4434.	2.8	22
137	He-atom scattering from MgO(100): calculating diffraction peak intensities with a semi ab initio potential. Physical Chemistry Chemical Physics, 2011, 13, 14750.	2.8	11
138	Electron correlation decides the stability of cubic versus hexagonal boron nitride. Physical Review B, 2011, 83, .	3.2	25
139	First-principles optical response of semiconductors and oxide materials. Physical Review B, 2011, 83, .	3.2	51
140	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.	2.5	169
141	Local MP2 with Density Fitting for Periodic Systems: A Parallel Implementation. Journal of Chemical Theory and Computation, 2011, 7, 2818-2830.	5.3	55
142	Electron Densities and Related Properties from the ab-initio Simulation of Crystalline Solids. , 2011, , 79-132.		3
143	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
144	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

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145	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.	3.0	49
146	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.	2.5	31
147	Polarizability and hyperpolarizability of BN zigzag nanotubes calculated by the coupled perturbed Kohn-Sham scheme. Physical Review B, 2011, 83, .	3.2	23
148	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.	0.8	52
149	ed 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.	2.6	19
150	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.	3.3	112
151	Pressure-induced transitions in solid nitrogen: Role of dispersive interactions. Physical Review B, 2011, 84, .	3.2	32
152	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, .	3.2	26
153	Periodic quantum mechanical simulation of the Heâ€“MgO(100) interaction potential. Journal of Chemical Physics, 2011, 134, 014706.	3.0	34
154	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.	3.0	24
155	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
156	Ab initio periodic study of the conformational behavior of glycine helical homopeptides. Journal of Computational Chemistry, 2010, 31, 1777-1784.	3.3	11
157	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.	2.0	121
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