Roberto Dovesi

List of Publications by Year
in descending order

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239 papers	16,841 citations	18482 62 h-index	16650 123 g-index
242 all docs	242 docs citations	242 times ranked	9317 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	Hartree-Fock Ab Initio Treatment of Crystalline Systems. Lecture Notes in Quantum Chemistry II, 1988, , .	0.3	577
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	Hartreeâ€“Fock geometry optimisation of periodic systems with the Crystal code. Chemical Physics Letters, 2001, 348, 131-138.	2.6	294
8	Theoretical study of electronic, magnetic, and structural properties of Î±-Fe2O3(hematite). Physical Review B, 1995, 51, 7441-7450.	3.2	273
9	The calculation of static polarizabilities of 1â€3D periodic compounds. the implementation in the crystal code. Journal of Computational Chemistry, 2008, 29, 1450-1459.	3.3	253
10	Electronic structure and stability of different crystal phases of magnesium oxide. Physical Review B, 1986, 33, 1308-1316.	3.2	240
11	Ab initio approach to molecular crystals: A periodic Hartreeâ€“Fock study of crystalline urea. Journal of Chemical Physics, 1990, 92, 7402-7411.	3.0	220
12	Exact-exchange Hartree-Fock calculations for periodic systems. I. Illustration of the method. International Journal of Quantum Chemistry, 1980, 17, 501-516.	2.0	214
13	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
14	Realistic Models of Hydroxylated Amorphous Silica Surfaces and MCMâ€41 Mesoporous Material Simulated by Largeâ€scale Periodic B3LYP Calculations. Advanced Materials, 2008, 20, 4579-4583.	21.0	199
15	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.	3.0	199
16	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
17	Ab-initio prediction of materials properties with CRYSTAL: MOF-5 as a case study. CrystEngComm, 2006, 8, 364-371.	2.6	187
18	Coupled perturbed Hartree-Fock for periodic systems: The role of symmetry and related computational aspects. Journal of Chemical Physics, 2008, 128, 014110.	3.0	186

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19	The vibrational spectrum of calcite (CaCO3): an ab initio quantum-mechanical calculation. Physics and Chemistry of Minerals, 2004, 31, 559-564.	0.8	182
20	Local-MP2 electron correlation method for nonconducting crystals. Journal of Chemical Physics, 2005, 122, 094113.	3.0	182
21	Ab-initio calculation of elastic constants of crystalline systems with the CRYSTAL code. Computer Physics Communications, 2009, 180, 1753-1759.	7.5	178
22	The Performance of Hybrid Density Functionals in Solid State Chemistry. Structure and Bonding, 2004, , 171-232.	1.0	171
23	Quantum-mechanical calculation of the solid-state equilibrium MgO+Î±-Al2O3â‡„MgAl2O4(spinel) versus pressure. Physical Review B, 1994, 49, 14179-14187.	3.2	169
24	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
25	On the electrostatic potential in crystalline systems where the charge density is expanded in Gaussian functions. Molecular Physics, 1992, 77, 629-665.	1.7	167
26	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
27	Spontaneous polarization as a Berry phase of the Hartree-Fock wave function: The case ofKNbO3. Physical Review B, 1997, 56, 10105-10114.	3.2	151
28	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
29	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
30	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
31	Large-Scale Condensed Matter DFT Simulations: Performance and Capabilities of the CRYSTAL Code. Journal of Chemical Theory and Computation, 2017, 13, 5019-5027.	5.3	138
32	The CRYSTAL code, 1976â€“2020 and beyond, a long story. Journal of Chemical Physics, 2020, 152, 204111.	3.0	133
33	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
34	Treatment of Coulomb interactions in Hartree-Fock calculations of periodic systems. Physical Review B, 1983, 28, 5781-5792.	3.2	127
35	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
36	Anab InitioHartreeâ^'Fock Study of the Cubic and Tetragonal Phases of Bulk Tungsten Trioxide. Journal of the American Chemical Society, 1996, 118, 12174-12182.	13.7	120

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37	Ab Initio Quantum Simulation in Solid State Chemistry. Reviews in Computational Chemistry, 2005, , 1-125.	1.5	120
38	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
39	Ab initio vibrational spectra and dielectric properties of carbonates: magnesite, calcite and dolomite. Theoretical Chemistry Accounts, 2007, 117, 991-1000.	1.4	108
40	Electronic, magnetic and crystal structure of Cr 2 O 3 by theoretical methods. Journal of Physics and Chemistry of Solids, 1996, 57, 1735-1741.	4.0	106
41	Analytical Hartree?Fock gradients with respect to the cell parameter for systems periodic in three dimensions. Theoretical Chemistry Accounts, 2004, 112, 394-402.	1.4	102
42	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
43	Ab initioHartree-Fock calculations of CaO, VO, MnO and NiO. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1993, 68, 653-666.	0.6	95
44	Exact-exchange Hartree-Fock calculations for periodic systems. II. Results for graphite and hexagonal boron nitride. International Journal of Quantum Chemistry, 1980, 17, 517-529.	2.0	93
45	Quantum mechanical calculation of the OH vibrational frequency in crystalline solids. Molecular Physics, 2005, 103, 2549-2558.	1.7	93
46	The vibrational spectrum of CaCO3 aragonite: A combined experimental and quantum-mechanical investigation. Journal of Chemical Physics, 2013, 138, 014201.	3.0	92
47	Characterization of the electronic structure of crystalline compounds through their localized Wannier functions. Journal of Chemical Physics, 2002, 116, 1120-1127.	3.0	87
48	Ab initio simulation of the IR spectra of pyrope, grossular, and andradite. Journal of Computational Chemistry, 2008, 29, 2268-2278.	3.3	84
49	The electronic structure of Î±â€quartz: A periodic Hartreeâ€“Fock calculation. Journal of Chemical Physics, 1987, 86, 6967-6971.	3.0	83
50	Magnetic interactions and the cooperative Jahn-Teller effect inKCuF3. Physical Review B, 1995, 52, 10150-10159.	3.2	83
51	A periodic ab initio extended basis set study of Î±-Al2O3. Molecular Physics, 1991, 72, 267-277.	1.7	82
52	Quantum Mechnical Hartreeâ€Fock Study of the Elastic Properties of Li₂S and Na₂S. Physica Status Solidi (B): Basic Research, 1993, 177, 157-163.	1.5	82
53	Electronic and magnetic structure ofKNiF3perovskite. Physical Review B, 1995, 52, 2381-2389.	3.2	79
54	Correlation correction to the Hartree-Fock total energy of solids. Physical Review B, 1987, 36, 891-897.	3.2	75

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55	On how differently the quasi-harmonic approximation works for two isostructural crystals: Thermal properties of periclase and lime. Journal of Chemical Physics, 2015, 142, 044114.	3.0	72
56	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
57	The vibrational frequencies of forsterite Mg2SiO4: an all-electron ab initio study with the CRYSTAL code. Physics and Chemistry of Minerals, 2006, 33, 383-393.	0.8	69
58	Infrared Spectra of Hydrogen-Bonded Ionic Crystals:Â Ab Initio Study of Mg(OH)2and Î²-Be(OH)2. Journal of Physical Chemistry B, 2004, 108, 13632-13637.	2.6	68
59	The Vibrational Spectrum of Î±-AlOOH Diaspore:â€‰ An Ab Initio Study with the CRYSTAL Code. Journal of Physical Chemistry B, 2007, 111, 9337-9346.	2.6	66
60	High pressure elastic properties of minerals from ab initio simulations: The case of pyrope, grossular and andradite silicate garnets. Journal of Chemical Physics, 2014, 140, 124703.	3.0	66
61	Adsorption energies of NH3 and NH+4 in zeolites corrected for the longâ€range electrostatic potential of the crystal. Journal of Chemical Physics, 1994, 101, 5865-5874.	3.0	65
62	Structural, electronic and magnetic properties of KMF3(M=Mn, Fe, Co, Ni). Faraday Discussions, 1997, 106, 173-187.	3.2	64
63	Coupled perturbed Kohn-Sham calculation of static polarizabilities of periodic compounds. Journal of Physics: Conference Series, 2008, 117, 012016.	0.4	63
64	Mechanical and molecular properties of ice VIII from crystalâ€orbital ab initio calculations. Journal of Chemical Physics, 1994, 100, 2128-2138.	3.0	61
65	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
66	Treatment of the exchange interactions in Hartree-Fock LCAO calculations of periodic systems. The Journal of Physical Chemistry, 1988, 92, 909-913.	2.9	60
67	Beryllium Oxide Nanotubes and their Connection to the Flat Monolayer. Journal of Physical Chemistry C, 2013, 117, 12864-12872.	3.1	60
68	First-principles study of the mechanisms of the pressure-induced dielectric anomalies in ferroelectric perovskites. Phase Transitions, 2013, 86, 1069-1084.	1.3	57
69	The structural, electronic and vibrational properties of LiOH and NaOH: an ab initio study. Chemical Physics Letters, 2004, 387, 453-459.	2.6	54
70	Ab initio quantum mechanical study of Î³-AlOOH boehmite: structure and vibrational spectrum. Physics and Chemistry of Minerals, 2009, 36, 47-59.	0.8	54
71	Ab initiostudy of antiferromagnetic rutile-typeFeF2. Physical Review B, 1995, 52, 2422-2427.	3.2	53
72	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

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73	Vibrational Spectrum of Katoite Ca3Al2[(OH)4]3:Â A Periodic ab Initio Study. Journal of Physical Chemistry B, 2006, 110, 692-701.	2.6	53
74	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.	3.3	52
75	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
76	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
77	First-principles optical response of semiconductors and oxide materials. Physical Review B, 2011, 83, .	3.2	51
78	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
79	Well localized crystalline orbitals obtained from Bloch functions:â€ƒThe case ofKNbO3. Physical Review B, 2001, 64, .	3.2	50
80	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
81	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
82	A quantum mechanical study of the perovskite structure type of MgSiO3. Physics and Chemistry of Minerals, 1993, 20, 407.	0.8	48
83	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
84	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.	2.0	47
85	On the electrostatic potential in linear periodic polymers. Computer Physics Communications, 1994, 84, 156-172.	7.5	47
86	Analytical Hartreeâ€“Fock gradients with respect to the cell parameter: systems periodic in one and two dimensions. Theoretical Chemistry Accounts, 2006, 115, 354-360.	1.4	47
87	CRYSTAL and EMBED, two computational tools for the ab initio study of electronic properties of crystals. International Journal of Quantum Chemistry, 2000, 77, 1032-1048.	2.0	46
88	Ab initiostudy ofMF2(M=Mn,Fe,Co,Ni)rutile-type compounds using the periodic unrestricted Hartree-Fock approach. Physical Review B, 2000, 62, 7816-7823.	3.2	46
89	Vibration Frequencies of Ca3Fe2Si3O12Andradite:Â An ab Initio Study with the CRYSTAL Code. Journal of Physical Chemistry B, 2005, 109, 18522-18527.	2.6	46
90	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.	2.6	46

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91	Near-Hartree-Fock wave functions for solids: The case of crystalline silicon. International Journal of Quantum Chemistry, 1992, 42, 5-33.	2.0	44
92	Periodic unrestricted Hartree-Fock study of corundumlikeTi2O3andV2O3. Physical Review B, 1997, 55, 16122-16131.	3.2	44
93	Hydrogarnet defect in chabazite and sodalite zeolites: A periodic Hartreeâ€“Fock and B3-LYP study. Journal of Chemical Physics, 2002, 117, 5337-5346.	3.0	44
94	The vibration properties of the (n,0) boron nitride nanotubes from ab initio quantum chemical simulations. Journal of Chemical Physics, 2013, 138, 054906.	3.0	44
95	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.	3.0	43
96	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
97	Fcenter in LiF: A quantum mechanicalab initioinvestigation of the hyperfine interaction between the unpaired electron at the vacancy and its first seven neighbors. Physical Review B, 2001, 63, .	3.2	42
98	B3LYP Simulation of the Full Vibrational Spectrum of 45S5 Bioactive Silicate Glass Compared to v-Silica. Chemistry of Materials, 2008, 20, 5610-5621.	6.7	42
99	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.	2.0	42
100	Substitutional nitrogen in diamond: A quantum mechanical investigation of the electronic and spectroscopic properties. Carbon, 2018, 134, 354-365.	10.3	42
101	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
102	Photoelasticity of crystals from theoretical simulations. Physical Review B, 2013, 88, .	3.2	41
103	Raman spectrum of NaAlSi₂O₆ jadeite. A quantum mechanical simulation. Journal of Raman Spectroscopy, 2014, 45, 703-709.	2.5	41
104	Periodic density functional theory and local-MP2 study of the librational modes of Ice XI. Journal of Chemical Physics, 2009, 130, 074505.	3.0	39
105	Detailed ab-initio analysis of the magnetic coupling in CuF2. Chemical Physics Letters, 2000, 319, 625-630.	2.6	37
106	Ab initio study of the cation vacancy at the surface and in bulk MgO. Physical Chemistry Chemical Physics, 2000, 2, 3893-3901.	2.8	37
107	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
108	Magnetic coupling in the weak ferromagnetCuF2. Physical Review B, 1999, 59, 1016-1023.	3.2	36

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109	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.	2.0	36
110	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
111	Structural and elastic anisotropy of crystals at high pressures and temperatures from quantum mechanical methods: The case of Mg2SiO4 forsterite. Journal of Chemical Physics, 2015, 142, 204502.	3.0	36
112	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
113	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
114	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
115	Correlation correction to the Hartree-Fock total energy of solids. II. Physica Scripta, 1988, 38, 194-198.	2.5	31
116	A quantum mechanical investigation of the electronic and magnetic properties of perovskite. Journal of Physics Condensed Matter, 1997, 9, 489-498.	1.8	31
117	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
118	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
119	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
120	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
121	Anharmonic Thermal Oscillations of the Electron Momentum Distribution in Lithium Fluoride. Physical Review Letters, 2015, 115, 117402.	7.8	30
122	Zinc oxide nanotubes: An ab initio investigation of their structural, vibrational, elastic, and dielectric properties. Journal of Chemical Physics, 2013, 138, 214706.	3.0	29
123	Quantum-Mechanical ab Initio Simulation of the Raman and IR Spectra of Fe₃Al₂Si₃O₁₂ Almandine. Journal of Physical Chemistry A, 2009, 113, 11289-11294.	2.5	28
124	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
125	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
126	In silico infrared and Raman spectroscopy under pressure: The case of CaSnO3 perovskite. Journal of Chemical Physics, 2015, 142, 014505.	3.0	28

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127	On the structural, electronic and magnetic properties of spinel. Journal of Physics Condensed Matter, 1997, 9, 10715-10724.	1.8	27
128	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
129	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
130	Comparison of different approaches to the study of local defects in crystals. I. Theoretical considerations and computational schemes. Physica Status Solidi (B): Basic Research, 1983, 116, 249-259.	1.5	26
131	Superexchange interaction in K2NiF4: an ab initio Hartree-Fock study. Journal of Physics Condensed Matter, 1995, 7, 7997-8007.	1.8	26
132	Phonon vibrational frequencies and elastic properties of solid SrFCl. An ab initio study. European Physical Journal B, 2005, 43, 453-461.	1.5	26
133	Single-layered chrysotile nanotubes: A quantum mechanical ab initio simulation. Journal of Chemical Physics, 2009, 131, 204701.	3.0	26
134	The electronic states of the neutral vacancy in diamond: a quantum mechanical approach. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	26
135	Lithium trapped-hole centre in magnesium oxide. An ab initio supercell study. Journal of Physics and Chemistry of Solids, 1998, 59, 7-12.	4.0	25
136	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
137	Quantum-mechanical calculation of the vibrational spectrum of beryl (Al4Be6Si12O36) at the Î“ point. Physics and Chemistry of Minerals, 2006, 33, 519-532.	0.8	24
138	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
139	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
140	Piezo-optic tensor of crystals from quantum-mechanical calculations. Journal of Chemical Physics, 2015, 143, 144504.	3.0	23
141	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
142	A quantum-mechanical study of the relative stability under pressure of MgSiO3-ilmenite, MgSiO3-perovskite, and MgO-periclase+SiO2-stishovite assemblage. Physics and Chemistry of Minerals, 1994, 21, 285.	0.8	22
143	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
144	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

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145	Elucidating the fundamental forces in protein crystal formation: the case of crambin. Chemical Science, 2016, 7, 1496-1507.	7.4	21
146	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
147	The VN₃H defect in diamond: a quantum-mechanical characterization. Physical Chemistry Chemical Physics, 2017, 19, 22221-22229.	2.8	20
148	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
149	Ab initio quantumâ€mechanical simulation of the Raman spectrum of grossular. Journal of Raman Spectroscopy, 2009, 40, 416-418.	2.5	19
150	Quantum-mechanical ab initio simulation of the Raman and IR spectra of Mn3Al2Si3O12 spessartine. Physics and Chemistry of Minerals, 2009, 36, 415-420.	0.8	19
151	Structure and Stability of the Al(OH)₃ Polymorphs Doyleite and Nordstrandite: A Quantum Mechanical ab Initio Study with the CRYSTAL06 Code. Journal of Physical Chemistry C, 2009, 113, 6785-6791.	3.1	19
152	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
153	"The infrared spectrum of spessartine" 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
154	Calculation of the dynamic first electronic hyperpolarizability Î²(â^'Ï‰ Ïƒ; Ï‰1,) Tj ETQq0 0 0 rgBT /Overlock Chemical Physics, 2015, 143, 244102.	3.0	19
155	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
156	Hartreeâ€“Fock study of polysulphurâ€nitride. I. The isolated infinite chain. Journal of Chemical Physics, 1984, 81, 2839-2844.	3.0	18
157	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.	3.0	18
158	Hydrogen atoms in the diamond vacancy defect. A quantum mechanical vibrational analysis. Carbon, 2018, 129, 349-356.	10.3	18
159	Vibrational spectroscopy of hydrogens in diamond: a quantum mechanical treatment. Physical Chemistry Chemical Physics, 2018, 20, 11930-11940.	2.8	17
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