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	The NV0 defects in diamond: A quantum mechanical characterization through its vibrational and Electron Paramagnetic Resonance spectroscopies. Journal of Physics and Chemistry of Solids, 2022, 160, 110304.	4.0	3
2	The superexchange mechanism in crystalline compounds. The case of KMF₃ (M = Mn, Fe, Co,) Tj ETQq0 0 0 rgBT /Overlock	1.8	3
3	Strategies for the optimization of the structure of crystalline compounds. Journal of Computational Chemistry, 2022, 43, 184-196.	3.3	9
4	The calculated energies and charge and spin distributions of the excited GR1 state in diamond. Journal of Chemical Physics, 2022, 156, 044708.	3.0	7
5	Quantum mechanical simulation of various phases of KVF₃ perovskite. Journal of Physics Condensed Matter, 2022, 34, 285401.	1.8	2
6	The role of spin density for understanding the superexchange mechanism in transition metal ionic compounds. The case of KMF₃ (M = Mn, Fe, Co, Ni, Cu) perovskites. Physical Chemistry Chemical Physics, 2022, 24, 12950-12960.	2.8	2
7	Self-trapped excitons in diamond: A Î”-SCF approach. Journal of Chemical Physics, 2022, 157, .	3.0	3
8	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
9	Interstitial carbon defects in silicon. A quantum mechanical characterization through the infrared and Raman spectra. Journal of Computational Chemistry, 2021, 42, 806-817.	3.3	2
10	Oxygen and vacancy defects in silicon. A quantum mechanical characterization through the IR and Raman spectra. Journal of Chemical Physics, 2021, 154, 174707.	3.0	4
11	A promising carbon-based nanosheet as a suitable Na-anode material. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2021, 268, 115121.	3.5	9
12	Vibrational Analysis of Paraelectricâ€“Ferroelectric Transition of LiNbO3: An Ab-Initio Quantum Mechanical Treatment. Symmetry, 2021, 13, 1650.	2.2	2
13	The NVâ¯â‹¯N+ charged pair in diamond: a quantum-mechanical investigation. Physical Chemistry Chemical Physics, 2021, 23, 18724-18733.	2.8	2
14	The ferromagnetic and anti-ferromagnetic phases (cubic, tetragonal, orthorhombic) of KMnF₃. A quantum mechanical investigation. Physical Chemistry Chemical Physics, 2021, 23, 26780-26792.	2.8	7
15	The effect of charge and spin state on the Infrared spectra and hyperfine coupling constants of point defects in Silicon. Physica B: Condensed Matter, 2021, 626, 413499.	2.7	0
16	Characterization of the negatively charged NV defect through the spin density distribution and the hyperfine coupling constants. Journal of Physics and Chemistry of Solids, 2021, , 110506.	4.0	0
17	The VN2 negatively charged defect in diamond. A quantum mechanical investigation of the EPR response. Carbon, 2020, 159, 443-450.	10.3	17
18	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

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19	From anisotropy of dielectric tensors to birefringence: a quantum mechanics approach. Rendiconti Lincei, 2020, 31, 835-851.	2.2	3
20	The VN defect in diamond: A quantum mechanical simulation of the vibrational spectra and EPR properties. Carbon, 2020, 170, 600-605.	10.3	5
21	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
22	Microscopic Characterization of Oxygen Defects in Diamond as Models for N3 and OK1 Defects: A Comparison of Calculated and Experimental Electron Paramagnetic Resonance Data. Journal of Physical Chemistry A, 2020, 124, 8263-8272.	2.5	2
23	Predicted strong spin-phonon interactions in Li-doped diamond. Physical Chemistry Chemical Physics, 2020, 22, 20612-20617.	2.8	5
24	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
25	The CRYSTAL code, 1976â€“2020 and beyond, a long story. Journal of Chemical Physics, 2020, 152, 204111.	3.0	133
26	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
27	An all-electron study of the low-lying excited states and optical constants of Al₂O₃ in the range 5â€“80 eV. Journal of Physics Condensed Matter, 2020, 32, 085901.	1.8	8
28	The spectroscopic characterization of interstitial oxygen in bulk silicon: A quantum mechanical simulation. Journal of Chemical Physics, 2020, 152, 054502.	3.0	5
29	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
30	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
31	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
32	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
33	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
34	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
35	Substitutional boron and nitrogen pairs in diamond. A quantum mechanical vibrational analysis. Carbon, 2019, 146, 709-716.	10.3	10
36	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

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37	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
38	Quantumâ€mechanical condensed matter simulations with CRYSTAL. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1360.	14.6	1,277
39	Experimental and Theoretical Infrared Signatures of REMO₃ (RE = La, Pr, Nd, Sm, and M =) Tj ETQq1 1 0.784314 rgBT /Ov	3.1	8
40	Vibrational spectroscopy of hydrogens in diamond: a quantum mechanical treatment. Physical Chemistry Chemical Physics, 2018, 20, 11930-11940.	2.8	17
41	Substitutional nitrogen in diamond: A quantum mechanical investigation of the electronic and spectroscopic properties. Carbon, 2018, 134, 354-365.	10.3	42
42	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
43	Hydrogen atoms in the diamond vacancy defect. A quantum mechanical vibrational analysis. Carbon, 2018, 129, 349-356.	10.3	18
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	The Infrared spectrum of very large (periodic) systems: global versus fragment strategiesâ€"the case of three defects in diamond. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	10
46	Scalars, vectors and tensors evolving from slabs to bulk. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	0
47	Low energy excitations in NiO based on a direct Î”-SCF approach. Journal of Physics Condensed Matter, 2018, 30, 495901.	1.8	16
48	Hydrogen, boron and nitrogen atoms in diamond: a quantum mechanical vibrational analysis. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	16
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	Scientific outline of Claudio Zicovich-Wilson. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	0
51	Comparison between cluster and supercell approaches: the case of defects in diamond. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	13
52	The A-center defect in diamond: quantum mechanical characterization through the infrared spectrum. Physical Chemistry Chemical Physics, 2017, 19, 14478-14485.	2.8	16
53	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
54	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

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55	The VN₃H defect in diamond: a quantum-mechanical characterization. Physical Chemistry Chemical Physics, 2017, 19, 22221-22229.	2.8	20
56	On the Use of Benchmarks for Multiple Properties. Computation, 2016, 4, 20.	2.0	7
57	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
58	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
59	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
60	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
61	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
62	The electronic states of the neutral vacancy in diamond: a quantum mechanical approach. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	26
63	Elucidating the fundamental forces in protein crystal formation: the case of crambin. Chemical Science, 2016, 7, 1496-1507.	7.4	21
64	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
65	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
66	Anharmonic Thermal Oscillations of the Electron Momentum Distribution in Lithium Fluoride. Physical Review Letters, 2015, 115, 117402.	7.8	30
67	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
68	Piezo-optic tensor of crystals from quantum-mechanical calculations. Journal of Chemical Physics, 2015, 143, 144504.	3.0	23
69	Quantum-mechanical simulation of the IR reflectance spectrum of Mn3Al2Si3O12 spessartine. , 2015, , .		0
70	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
71	In silico infrared and Raman spectroscopy under pressure: The case of CaSnO3 perovskite. Journal of Chemical Physics, 2015, 142, 014505.	3.0	28
72	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

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73	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
74	Structure and Vibrational Spectraâ˜†. , 2015, , .		0
75	Pressure effect on elastic anisotropy of crystals from ab initio simulations: The case of silicate garnets. Journal of Chemical Physics, 2014, 140, 234703.	3.0	15
76	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
77	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
78	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
79	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
80	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
81	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
82	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
83	Elasticity of grossularâ€“andradite solid solution: an ab initio investigation. Physical Chemistry Chemical Physics, 2014, 16, 15331.	2.8	16
84	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
85	Raman spectrum of NaAlSi₂O₆ jadeite. A quantum mechanical simulation. Journal of Raman Spectroscopy, 2014, 45, 703-709.	2.5	41
86	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
87	Photoelasticity of crystals from theoretical simulations. Physical Review B, 2013, 88, .	3.2	41
88	Anomalous birefringence in andraditeâ€“grossular solid solutions: a quantum-mechanical approach. Physics and Chemistry of Minerals, 2013, 40, 781-788.	0.8	9
89	Structure and Vibrational Spectra. , 2013, , 971-987.		1
90	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

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91	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
92	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
93	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
94	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
95	First-principles study of the mechanisms of the pressure-induced dielectric anomalies in ferroelectric perovskites. Phase Transitions, 2013, 86, 1069-1084.	1.3	57
96	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
97	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
98	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
99	The electronic structure of MgO nanotubes. An ab initio quantum mechanical investigation. Physical Chemistry Chemical Physics, 2013, 15, 13296.	2.8	10
100	The infrared vibrational spectrum of andradite-grossular solid solutions: A quantum mechanical simulation. American Mineralogist, 2013, 98, 966-976.	1.9	13
101	Beryllium Oxide Nanotubes and their Connection to the Flat Monolayer. Journal of Physical Chemistry C, 2013, 117, 12864-12872.	3.1	60
102	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
103	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
104	The vibrational spectrum of CaCO3 aragonite: A combined experimental and quantum-mechanical investigation. Journal of Chemical Physics, 2013, 138, 014201.	3.0	92
105	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
106	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
107	On the use of symmetry in SCF calculations. The case of fullerenes and nanotubes. AIP Conference Proceedings, 2012, , .	0.4	9
108	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

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109	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
110	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
111	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
112	First-principles optical response of semiconductors and oxide materials. Physical Review B, 2011, 83, .	3.2	51
113	Electron Densities and Related Properties from the ab-initio Simulation of Crystalline Solids. , 2011, , 79-132.		3
114	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
115	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
116	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
117	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, 713-728.	0.8	52
118	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.	2.6	19
119	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
120	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
121	Ab initio periodic study of the conformational behavior of glycine helical homopeptides. Journal of Computational Chemistry, 2010, 31, 1777-1784.	3.3	11
122	Ab initio quantumâ€mechanical prediction of the IR and Raman spectra of Ca₃Cr₂Si₃O₁₂ Uvarovite garnet. International Journal of Quantum Chemistry, 2010, 110, 416-421.	2.0	14
123	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
124	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
125	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
126	Magnetic interactions in Ca₃Fe₂Ge₃O₁₂ and Ca₃Cr₂Ge₃O₁₂ garnets. An ab initio allâ€electron quantum mechanical simulation. International Journal of Quantum Chemistry, 2010, 110, 2192-2201.	2.0	6

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127	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
128	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
129	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
130	Ab initio modeling of layered materials with the CRYSTAL code: an overview. Zeitschrift FÃ¼r Kristallographie, 2009, 224, 241-250.	1.1	8
131	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
132	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
133	Ab initio quantumâ€mechanical simulation of the Raman spectrum of grossular. Journal of Raman Spectroscopy, 2009, 40, 416-418.	2.5	19
134	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
135	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
136	Ab-initio calculation of elastic constants of crystalline systems with the CRYSTAL code. Computer Physics Communications, 2009, 180, 1753-1759.	7.5	178
137	Single-layered chrysotile nanotubes: A quantum mechanical ab initio simulation. Journal of Chemical Physics, 2009, 131, 204701.	3.0	26
138	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
139	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
140	Andraditeâ€“Uvarovite Solid Solutions. An ab Initio All-Electron Quantum Mechanical Simulation with the CRYSTAL06 Code. Journal of Physical Chemistry C, 2009, 113, 14507-14511.	3.1	14
141	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
142	Ab initio simulation of the IR spectra of pyrope, grossular, and andradite. Journal of Computational Chemistry, 2008, 29, 2268-2278.	3.3	84
143	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
144	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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145	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
146	Ab-initioquantum mechanical study of akdalaite (5Al₂O₃Â·) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 707 012013.	0.4	12
147	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
148	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
149	Coupled perturbed Kohn-Sham calculation of static polarizabilities of periodic compounds. Journal of Physics: Conference Series, 2008, 117, 012016.	0.4	63
150	Comparison of the polarizability of periodic systems computed by using the length and velocity operators. Journal of Physics: Conference Series, 2008, 117, 012023.	0.4	14
151	Coupled Perturbed Hartree-Fock Calculation of the Static Polarizability for Periodic Systems: Implementation in the CRYSTAL Code. AIP Conference Proceedings, 2007, , .	0.4	13
152	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
153	Ab initio vibrational spectra and dielectric properties of carbonates: magnesite, calcite and dolomite. Theoretical Chemistry Accounts, 2007, 117, 991-1000.	1.4	108
154	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
155	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
156	Ab-initio prediction of materials properties with CRYSTAL: MOF-5 as a case study. CrystEngComm, 2006, 8, 364-371.	2.6	187
157	The anisotropy of dielectric properties in the orthorhombic and hexagonal structures of Anhydrite â€“ anab initio and hybrid DFT study. Physica Status Solidi (B): Basic Research, 2006, 243, 2935-2951.	1.5	7
158	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
159	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
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