Michel RÃ©rat

List of Publications by Year
in descending order

163 papers	7,536 citations	101543 36 h-index	56724 83 g-index
166 all docs	166 docs citations	166 times ranked	6593 citing authors

#	Article	IF	Citations
1	RbCeX2 Crystal (X = S, Se, Te): Pressure-Induced Spin-Selective Gapless Transition and Response Properties. Journal of Alloys and Compounds, 2022, 898, 162760.	5.5	3
2	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
3	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
4	Electronic and magnetic properties of yttria-stabilized zirconia (6.7Âmol% in Y2O3) doped with Er3+ ions from first-principle computations. Journal of Materials Science, 2021, 56, 8014-8023.	3.7	0
5	First-Principles Calculation of the Optical Rotatory Power of Periodic Systems: Application on Î±-Quartz, Tartaric Acid Crystal, and Chiral (n,m)-Carbon Nanotubes. Journal of Chemical Theory and Computation, 2021, 17, 4063-4076.	5.3	13
6	Theoretical insight into electronic and optical behaviour of H-adsorbed Zn-terminated Zn3N2-(100)-non-polar surface. Vacuum, 2021, 192, 110467.	3.5	1
7	xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si24.svg"><mml:mrow><mml:msup><mml:mrow><mml:mo stretchy="false">(</mml:mo><mml:mi>Ï‡</mml:mi></mml:mrow><mml:mfenced open="(") Tj ETQq1 1 0.784314 rgBT /Overlock 10 T	2.6	1
8	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
9	From anisotropy of dielectric tensors to birefringence: a quantum mechanics approach. Rendiconti Lincei, 2020, 31, 835-851.	2.2	3
10	From Pyridine Adduct of Borabenzene to (In)finite Graphene Architectures Functionalized with N â† B Dative Bonds. Prototype Systems of Strong One- and Two-Photon Quantum Transitions Triggering Large Nonlinear Optical Responses. Journal of Physical Chemistry C, 2020, 124, 21063-21074.	3.1	9
11	The CRYSTAL code, 1976â€“2020 and beyond, a long story. Journal of Chemical Physics, 2020, 152, 204111.	3.0	133
12	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
13	Magnetic semiconductor properties of RbLnSe2 (LnÂ=ÂCe, Pr, Nd, Gd): A density functional study. Journal of Magnetism and Magnetic Materials, 2020, 501, 166448.	2.3	11
14	Computational analysis of strain-induced electronic and optical properties of Zn3As2. Journal of Materials Science, 2020, 55, 5099-5110.	3.7	5
15	Calculation of Anharmonic IR and Raman Intensities for Periodic Systems from DFT Calculations: Implementation and Validation. Journal of Chemical Theory and Computation, 2020, 16, 3343-3351.	5.3	7
16	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
17	Third-order nonlinear optical susceptibility of crystalline oxide yttria-stabilized zirconia. Photonics Research, 2020, 8, 110.	7.0	19
18	Polyaromatic Systems Combining Increasing Optical Gaps and Amplified Nonlinear Optical Properties. A Comprehensive Theoretical Study on B₃N₃ Doped Nanographenes. Journal of Physical Chemistry C, 2019, 123, 21135-21149.	3.1	11

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19	Structural, electronic and optical properties of ABTe2 (A = Li, Na, K, Rb, Cs and B = Sc, Y, La): Insights from first-principles computations. Journal of Solid State Chemistry, 2019, 279, 120954.	2.9	13
20	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
21	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
22	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
23	Determination of the Macroscopic Electric Susceptibilities Î§ (n) from the Microscopic (hyper)polarizabilities Î±, Î² and Î³. , 2019, , 771-774.		0
24	Quantumâ€mechanical condensed matter simulations with CRYSTAL. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1360.	14.6	1,277
25	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
26	Hydrogen atoms in the diamond vacancy defect. A quantum mechanical vibrational analysis. Carbon, 2018, 129, 349-356.	10.3	18
27	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
28	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
29	Scalars, vectors and tensors evolving from slabs to bulk. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	0
30	Structure prediction of nanoclusters from global optimization techniques: Computational strategies and connection to experiments. Computational and Theoretical Chemistry, 2017, 1107, 1.	2.5	0
31	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
32	BiVO3 : A Bi-based material with promising uv-visible light absorption properties. Physical Review B, 2017, 96, .	3.2	11
33	Establishing the pivotal role of local aromaticity in the electronic properties of boron-nitride graphene lateral hybrids. Physical Chemistry Chemical Physics, 2016, 18, 25315-25328.	2.8	19
34	Longitudinal and transverse hyperpolarizabilities of carbon nanotubes: a computational investigation through the coupled-perturbed Hartreeâ€“Fock/Kohnâ€“Sham scheme. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	6
35	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
36	Piezoelectricity of Functionalized Graphene: A Quantum-Mechanical Rationalization. Journal of Physical Chemistry C, 2016, 120, 7795-7803.	3.1	26

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37	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
38	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
39	The linear and nonlinear response of infinite periodic systems to static and/or dynamic electric fields. Implementation in CRYSTAL code. , 2015, , .		0
40	Dual luminescence in solid CuI(piperazine): hypothesis of an emissive 1-D delocalized excited state. Dalton Transactions, 2015, 44, 13003-13006.	3.3	24
41	Ab Initio Calculation of the Ultravioletâ€“Visible (UV-vis) Absorption Spectrum, Electron-Loss Function, and Reflectivity of Solids. Journal of Chemical Theory and Computation, 2015, 11, 3245-3258.	5.3	51
42	Inducing a Finite In-Plane Piezoelectricity in Graphene with Low Concentration of Inversion Symmetry-Breaking Defects. Journal of Physical Chemistry C, 2015, 119, 8966-8973.	3.1	33
43	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
44	Low-temperature phase of BaTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>: Piezoelectric, dielectric, elastic, and photoelastic properties fromab initiosimulations. Physical Review B, 2014, 89, .	3.2	60
45	Piezoelectric, elastic, structural and dielectric properties of the Si_{1â^'x}Ge_xO₂solid solution: a theoretical study. Journal of Physics Condensed Matter, 2014, 26, 205401.	1.8	14
46	Semiconductors Used in Photovoltaic and Photocatalytic Devices: Assessing Fundamental Properties from DFT. Journal of Physical Chemistry C, 2014, 118, 5997-6008.	3.1	239
47	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
48	Prediction of electronic (hyper)polarizabilities of titania nanotubes: A DFT periodic study. Computational Materials Science, 2013, 68, 280-286.	3.0	4
49	Structural and electronic properties of Sb-doped SnO2 (110) surface: A first principles study. Applied Surface Science, 2013, 284, 581-587.	6.1	25
50	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
51	First-principles study of the mechanisms of the pressure-induced dielectric anomalies in ferroelectric perovskites. Phase Transitions, 2013, 86, 1069-1084.	1.3	57
52	The electronic structure of MgO nanotubes. An ab initio quantum mechanical investigation. Physical Chemistry Chemical Physics, 2013, 15, 13296.	2.8	10
53	Piezoelectricity of SrTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>: Anab initiodescription. Physical Review B, 2013, 88, .	3.2	66
54	First principles calculations of magnetic properties of Rh-doped SnO2(110) surfaces. Applied Surface Science, 2013, 269, 41-44.	6.1	19

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55	Beryllium Oxide Nanotubes and their Connection to the Flat Monolayer. Journal of Physical Chemistry C, 2013, 117, 12864-12872.	3.1	60
56	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
57	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
58	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
59	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
60	Static and dynamic coupled perturbed Hartree-Fock vibrational (hyper)polarizabilities of polyacetylene calculated by the finite field nuclear relaxation method. Journal of Chemical Physics, 2012, 137, 014103.	3.0	6
61	Polarizability and charge density distribution in crystalline urea. AIP Conference Proceedings, 2012, , .	0.4	1
62	Response properties of AgCl and AgBr under an external static electric field: A density functional study. Solid State Sciences, 2012, 14, 1412-1418.	3.2	6
63	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
64	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
65	Ab initio electron energyâ€loss spectra and depolarization effects: Application to carbon nanotubes. International Journal of Quantum Chemistry, 2012, 112, 2171-2184.	2.0	1
66	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
67	First-principles optical response of semiconductors and oxide materials. Physical Review B, 2011, 83, .	3.2	51
68	Properties of Carbon Nanotubes: An ab Initio Study Using Large Gaussian Basis Sets and Various DFT Functionals. Journal of Physical Chemistry C, 2011, 115, 8876-8885.	3.1	42
69	Polarizability and hyperpolarizability of BN zigzag nanotubes calculated by the coupled perturbed Kohn-Sham scheme. Physical Review B, 2011, 83, .	3.2	23
70	Electronic and Optical Modeling of Solar Cell Compounds CuGaSe2 and CuInSe2. Journal of Electronic Materials, 2011, 40, 2197-2208.	2.2	31
71	Polarizabilities of carbon nanotubes: Importance of the crystalline orbitals relaxation in presence of an electric field. International Journal of Quantum Chemistry, 2011, 111, 797-806.	2.0	2
72	Structural, electronic, elastic, and piezoelectric properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-quartz and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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73	Brillouin Spectroscopy, Calculated Elastic and Bond Properties of GaAsO₄. Inorganic Chemistry, 2010, 49, 9470-9478.	4.0	13
74	Effect of crystal packing on the static polarizability and first-hyperpolarizability of crystalline urea: anab initiocomputational study. Acta Crystallographica Section A: Foundations and Advances, 2010, 66, s70-s70.	0.3	0
75	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
76	Response of low quartz<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu the presence of an external static electric field: A density functional theory study. Physical Review B, 2009, 80, .	3.2	18
77	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
78	First-principles study of the optical properties of BeO in its ambient and high-pressure phases. Journal of Physics and Chemistry of Solids, 2009, 70, 789-795.	4.0	62
79	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.	3.0	24
80	Polarization of one-dimensional periodic systems in a static electric field: Sawtooth potential treatment revisited. Journal of Chemical Physics, 2009, 131, 044109.	3.0	10
81	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
82	Electronic and optical properties under pressure effect of alkali metal oxides. European Physical Journal B, 2008, 64, 35-42.	1.5	33
83	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
84	Study of intercalated Ti atom in tetrahedral or octahedral sites of titanium disulfide (001) surfaces: Theoretical scanning tunneling microscopy images. Journal of Chemical Physics, 2008, 128, 014708.	3.0	2
85	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
86	Coupled perturbed Kohn-Sham calculation of static polarizabilities of periodic compounds. Journal of Physics: Conference Series, 2008, 117, 012016.	0.4	63
87	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
88	First-principles calculations of the elastic, electronic, and optical properties of the filled skutteruditesCeFe4P12andThFe4P12. Physical Review B, 2007, 75, .	3.2	66
89	Coupled Perturbed Hartree-Fock Calculation of the Static Polarizability for Periodic Systems: Implementation in the CRYSTAL Code. AIP Conference Proceedings, 2007, , .	0.4	13
90	Electronic and structural properties of Ti vacancies on the (001) surface of TiS2: Theoretical scanning tunneling microscopy images. Journal of Chemical Physics, 2007, 126, 074703.	3.0	3

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91	Ti vacancies on the (001) surface of TiS2 detected by scanning tunneling microscopy: A combined experimental and theoretical study. Solid State Sciences, 2007, 9, 594-599.	3.2	8
92	First-principles study of the structural, electronic, and optical properties ofGa2O3in its monoclinic and hexagonal phases. Physical Review B, 2006, 74, .	3.2	510
93	Structural, electronic, elastic and high-pressure properties of some alkaline-earth chalcogenides: An ab initio study. Physica B: Condensed Matter, 2006, 371, 12-19.	2.7	69
94	Elastic and optical properties of BeS, BeSe and BeTe under pressure. Solid-State Electronics, 2006, 50, 1382-1388.	1.4	73
95	Ab initiocalculations of the dispersion contribution to the physisorption potential: Application to theN2-BN system. Physical Review B, 2006, 73, .	3.2	7
96	Full-potential calculations of structural, elastic and electronic properties of MgAl2O4 and ZnAl2O4 compounds. Physics Letters, Section A: General, Atomic and Solid State Physics, 2005, 344, 271-279.	2.1	73
97	First-principles calculations of optical properties of GeC, SnC and GeSn under hydrostatic pressure. Physica B: Condensed Matter, 2005, 355, 392-400.	2.7	35
98	Structural, electronic and optical properties of fluorite-type compounds. European Physical Journal B, 2005, 47, 63-70.	1.5	31
99	Quasienergy Derivative Method for the Optical Susceptibilities of Molecules in the Floquet Theory. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2005, 99, 545.	0.6	0
100	First-principle calculations of structural, electronic and optical properties of BaTiO3 and BaZrO3 under hydrostatic pressure. Solid State Communications, 2005, 136, 120-125.	1.9	104
101	First-principles study of structural, electronic and optical properties of BaF2in its cubic, orthorhombic and hexagonal phases. Journal of Physics Condensed Matter, 2003, 15, 709-718.	1.8	30
102	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
103	First-principle study of structural, electronic and elastic properties of SrS, SrSe and SrTe under pressure. Physica B: Condensed Matter, 2003, 339, 208-215.	2.7	92
104	Intramolecular dependence of the frequency-dependent polarizabilities of K2(a3Î£u+) and van der Waals dispersion coefficients for X+K2, X2+K and X2+K2 (X=Li,Na,K). Computational and Theoretical Chemistry, 2003, 633, 137-144.	1.5	6
105	Full potential linearized augmented plane wave calculations of structural and electronic properties of GeC, SnC and GeSn. Physica B: Condensed Matter, 2003, 336, 321-328.	2.7	45
106	Floquet gauge-invariant coupled perturbation theory in calculations of the optical susceptibilities of molecules. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2003, 94, 496-501.	0.6	1
107	Intramolecular dependence of the frequency dependent polarizabilities of Li2(a 3Î£+ u) and Na2(a 3Î£+ u) and van der Waals dispersion coefficients for atom-diatom and diatom-diatom alkali dimers. Molecular Physics, 2003, 101, 373-380.	1.7	16
108	Theoretical determination of the ionization cross-section of water. Computational and Theoretical Chemistry, 2002, 577, 17-33.	1.5	4

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109	Ab initio calculation of excited state dipole polarizability - Application to the first 1, 3Î£+g,u states of Li 2. European Physical Journal D, 2001, 17, 329-335.	1.3	17
110	Ab initio calculations of the second dynamic hyperpolarizability of LiH by means of Floquet theory approach. European Physical Journal D, 2001, 15, 199-208.	1.3	11
111	Recovering experimental and theoretical electron densities in corundum using the multipolar model: IUCr Multipole Refinement Project. Acta Crystallographica Section A: Foundations and Advances, 2001, 57, 290-303.	0.3	46
112	Long-range dispersion coefficients for the low-lying electronic states of Mg2 from the calculation of the frequency-dependent dipole polarizabilities of Mg in its ground and excited states. Chemical Physics Letters, 2001, 334, 403-410.	2.6	8
113	Excited states dipole polarizabilities of calcium atom and long-range dispersion coefficients for the low-lying electronic states of Ca2 and CaMg. Chemical Physics Letters, 2001, 343, 397-403.	2.6	20
114	First-principles calculations of nonlinear optical susceptibility of inorganic materials. Journal of Physics Condensed Matter, 2001, 13, 343-351.	1.8	6
115	Dynamic dipole polarizabilities for the ground 41S and the low-lying 41,3P and 51,3S excited states of Zn. Calculation of long-range coefficients of Zn2. Journal of Physics B: Atomic, Molecular and Optical Physics, 2001, 34, 2313-2323.	1.5	16
116	A theoretical study of stability, electronic, and optical properties of GeC and SnC. Journal of Applied Physics, 2000, 88, 6462-6466.	2.5	81
117	Long-range coefficients for the low-lying electronic states of BeLi and Be2. Journal of Chemical Physics, 1999, 110, 2051-2058.	3.0	8
118	Dynamic dipole polarizabilities and C6 dispersion coefficients for small clusters of beryllium Be (n=2,3,4). Chemical Physics Letters, 1999, 301, 43-52.	2.6	7
119	Compton profiles and polarizability as two similar probes of the electronic structure of 14 electron diatomic molecules: An ab initio study. International Journal of Quantum Chemistry, 1999, 71, 63-74.	2.0	8
120	First-principles study of stability, band structure, and optical properties of the ordered Ge0.50Sn0.50 alloy. Applied Physics Letters, 1999, 75, 4127-4129.	3.3	48
121	Ab Initio Self-Consistent Calculations of the Polarizability and Related Functions of Cubic SiC. Journal of Physical Chemistry B, 1999, 103, 5441-5445.	2.6	5
122	Compton profiles and polarizability as two similar probes of the electronic structure of 14 electron diatomic molecules: An ab initio study. International Journal of Quantum Chemistry, 1999, 71, 63-74.	2.0	1
123	Theoretical treatment of the electronic circular dichroism spectrum and the optical rotatory power of H2S2. Chemical Physics, 1998, 226, 297-306.	1.9	29
124	A quantum-mechanical calculation of the dynamic structure factors of magnesium difluoride. International Journal of Quantum Chemistry, 1998, 58, 419-429.	2.0	4
125	Ab InitioCalculation of the Structure Factors and Compton Profiles of Cubic Silicon Carbide. Acta Crystallographica Section A: Foundations and Advances, 1998, 54, 1019-1027.	0.3	8
126	Dynamic dipole polarizabilities for a lithium isoelectronic series in their ground and two first doublet excited states. Journal of Chemical Physics, 1998, 108, 7060-7064.	3.0	11

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127	Ab initioself-consistent calculations of the Compton profiles and polarizabilities of diamond and cubic boron nitride. Journal of Physics Condensed Matter, 1998, 10, 557-575.	1.8	10
128	Dynamic scalar and tensor polarizabilities for the low-lying 2 and 2 states of Be. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, 5077-5084.	1.5	9
129	Ab initio calculations of dipole polarizabilities of Na and K in their 32D-state and determination of long-range coefficients for S+D molecular states of Na2, K2, and NaK. Journal of Chemical Physics, 1998, 109, 7246-7251.	3.0	10
130	Dipole polarizabilities of Na and long-range coefficients for various molecular states of Na2. Journal of Chemical Physics, 1997, 106, 3658-3662.	3.0	12
131	Frequency-dependent dipole and quadrupole polarizabilities for the ground state of boron. Journal of Physics B: Atomic, Molecular and Optical Physics, 1997, 30, 167-176.	1.5	12
132	Topology of potential hypersurfaces of two, three and four dipoles interacting at long distances. Journal of Mathematical Chemistry, 1997, 22, 235-247.	1.5	3
133	Ab initio calculation of dynamic polarizability and dielectric constant of carbon and silicon cubic crystals. Journal of Computational Chemistry, 1997, 18, 1253-1263.	3.3	27
134	Dipole Polarizabilities of Li, C, and O and Long-Range Coefficients for Various Molecular States of Li2, CO, and O2. Journal of Molecular Spectroscopy, 1997, 182, 260-270.	1.2	28
135	Dynamic polarizability and hyperpolarizability for the 14 electron molecules CO and BF. Chemical Physics Letters, 1997, 280, 203-211.	2.6	18
136	PolarisabilitÃ©s et hyperpolarisabilitÃ©s statiques et dynamiques de CO⁺ dans son Ã©tat fondamental (X²â^'⁺) Ã partir dâ€™un calcul ab-initio IC. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1997, 94, 1553-1567.	0.2	0
137	Long-range coefficients for the low-lying electronic states of LiB. Chemical Physics Letters, 1996, 257, 409-413.	2.6	11
138	Compton profiles of the isoelectronic BeO and BN molecules: an ab initio study. Chemical Physics Letters, 1996, 263, 767-774.	2.6	10
139	LCAO-LDA calculation of Compton profiles in hexagonal BN; comparison with experiments. Journal of Physics Condensed Matter, 1996, 8, 10425-10434.	1.8	2
140	Theoretical ab initio calculations of the structure factors of fluorite (CaF2). Acta Crystallographica Section A: Foundations and Advances, 1995, 51, 323-328.	0.3	8
141	Dynamic polarizabilities and van der Waals coefficients for the ground 22Sand excited 24Postates of Li. Physical Review A, 1994, 49, 2493-2497.	2.5	24
142	Dynamic scalar and tensor polarizabilities of the 21Pand 23Pstates of He. Physical Review A, 1994, 49, 829-832.	2.5	22
143	A quantum chemical method for the calculation of dynamic structure factors: Applications to silicon, magnesium oxide and beryllium oxide. Theoretica Chimica Acta, 1994, 89, 213-226.	0.8	10
144	Topological complexity of potential surfaces and application to C2H2 molecule. Theoretica Chimica Acta, 1994, 88, 285-298.	0.8	5

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145	Ab initio Hartreeâ€“Fock study of lithium and sodium sulfides: electronic and scattering properties. Acta Crystallographica Section B: Structural Science, 1994, 50, 279-290.	1.8	19
146	Ab initio Cl determination of electric moments and frequency dependent polarizabilities and hyperpolarizabilities for CO. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1994, 91, 1387-1400.	0.2	5
147	Topologie des plus Â« simples Â» surfaces de potentiel pour des micro-agrÃ©gats. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1994, 91, 1401-1418.	0.2	0
148	Elastic properties in BeO. An ab initio Hartree-Fock calculation. Chemical Physics Letters, 1993, 211, 249-254.	2.6	20
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