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	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	First-principles study of the structural, electronic, and optical properties ofGa2O3in its monoclinic and hexagonal phases. Physical Review B, 2006, 74, .	3.2	510
4	The calculation of static polarizabilities of 1â€3D periodic compounds. the implementation in the crystal code. Journal of Computational Chemistry, 2008, 29, 1450-1459.	3.3	253
5	Semiconductors Used in Photovoltaic and Photocatalytic Devices: Assessing Fundamental Properties from DFT. Journal of Physical Chemistry C, 2014, 118, 5997-6008.	3.1	239
6	Calculation of first and second static hyperpolarizabilities of one- to three-dimensional periodic compounds. Implementation in the <scp>CRYSTAL</scp> code.. Journal of Chemical Physics, 2008, 129, 244110.	3.0	199
7	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
8	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
9	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
10	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
11	The CRYSTAL code, 1976â€“2020 and beyond, a long story. Journal of Chemical Physics, 2020, 152, 204111.	3.0	133
12	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
13	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
14	Crystal structure and magnetic and EPR properties of the heterobinuclear complex CuNi(fsa)2en(H2O)2.H2O (H4(fsa)2en = N,N'-bis(2-hydroxy-3-carboxybenzylidene)-1,2,-diaminoethane). Inorganic Chemistry, 1982, 21, 3050-3059.	4.0	81
15	A theoretical study of stability, electronic, and optical properties of GeC and SnC. Journal of Applied Physics, 2000, 88, 6462-6466.	2.5	81
16	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
17	Elastic and optical properties of BeS, BeSe and BeTe under pressure. Solid-State Electronics, 2006, 50, 1382-1388.	1.4	73
18	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

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19	First-principles calculations of the elastic, electronic, and optical properties of the filled skutteruditesCeFe4P12andThFe4P12. Physical Review B, 2007, 75, .	3.2	66
20	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
21	Coupled perturbed Kohn-Sham calculation of static polarizabilities of periodic compounds. Journal of Physics: Conference Series, 2008, 117, 012016.	0.4	63
22	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
23	Beryllium Oxide Nanotubes and their Connection to the Flat Monolayer. Journal of Physical Chemistry C, 2013, 117, 12864-12872.	3.1	60
24	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
25	First-principles study of the mechanisms of the pressure-induced dielectric anomalies in ferroelectric perovskites. Phase Transitions, 2013, 86, 1069-1084.	1.3	57
26	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
27	First-principles optical response of semiconductors and oxide materials. Physical Review B, 2011, 83, .	3.2	51
28	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
29	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
30	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
31	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
32	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
33	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
34	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
35	Evaluating dynamic multipole polarizabilities and van der Waals dispersion coefficients of two-electron systems with a quantum Monte Carlo calculation: A comparison with someab	2.5	37
36	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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37	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
38	Performance of a gauge-invariant method on calculated dynamic polarizabilities. Physical Review A, 1992, 45, 6263-6267.	2.5	36
39	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
40	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
41	Electronic and optical properties under pressure effect of alkali metal oxides. European Physical Journal B, 2008, 64, 35-42.	1.5	33
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	Nonlinear optical properties of H2and D2. Journal of Chemical Physics, 1990, 92, 1902-1908.	3.0	31
44	Structural, electronic and optical properties of fluorite-type compounds. European Physical Journal B, 2005, 47, 63-70.	1.5	31
45	Electronic and Optical Modeling of Solar Cell Compounds CuGaSe2 and CuInSe2. Journal of Electronic Materials, 2011, 40, 2197-2208.	2.2	31
46	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
47	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
48	Theoretical treatment of the electronic circular dichroism spectrum and the optical rotatory power of H2S2. Chemical Physics, 1998, 226, 297-306.	1.9	29
49	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
50	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
51	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
52	Piezoelectricity of Functionalized Graphene: A Quantum-Mechanical Rationalization. Journal of Physical Chemistry C, 2016, 120, 7795-7803.	3.1	26
53	Structural and electronic properties of Sb-doped SnO2 (110) surface: A first principles study. Applied Surface Science, 2013, 284, 581-587.	6.1	25
54	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

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55	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
56	Dual luminescence in solid CuI(piperazine): hypothesis of an emissive 1-D delocalized excited state. Dalton Transactions, 2015, 44, 13003-13006.	3.3	24
57	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
58	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
59	Dynamic polarizabilities and van der Waals coefficients of the 21Sand 23Smetastable states of helium. Physical Review A, 1993, 48, 161-165.	2.5	23
60	Polarizability and hyperpolarizability of BN zigzag nanotubes calculated by the coupled perturbed Kohn-Sham scheme. Physical Review B, 2011, 83, .	3.2	23
61	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
62	Dynamic scalar and tensor polarizabilities of the 21Pand 23Pstates of He. Physical Review A, 1994, 49, 829-832.	2.5	22
63	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
64	Higherâ€order polarizabilities for the helium isoelectronic series. Journal of Chemical Physics, 1989, 91, 5489-5491.	3.0	21
65	Calculation of dynamic polarizabilities with a multideterminental ket including a dipole-moment factor: Extrapolation method and application toLi2, LiH, and CO. Physical Review A, 1991, 43, 5832-5846.	2.5	21
66	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
67	Electric field variant ket for the calculation of dynamic polarizabilities. Application to H2O and N2. International Journal of Quantum Chemistry, 1989, 36, 169-178.	2.0	20
68	Time-dependent gauge-invariant approach to the calculation of dynamic hyperpolarizabilities: Application to FH and LiH. Physical Review A, 1992, 46, 5471-5477.	2.5	20
69	Elastic properties in BeO. An ab initio Hartree-Fock calculation. Chemical Physics Letters, 1993, 211, 249-254.	2.6	20
70	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
71	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
72	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

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73	First principles calculations of magnetic properties of Rh-doped SnO2(110) surfaces. Applied Surface Science, 2013, 269, 41-44.	6.1	19
74	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
75	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
76	Third-order nonlinear optical susceptibility of crystalline oxide yttria-stabilized zirconia. Photonics Research, 2020, 8, 110.	7.0	19
77	Dynamic polarizability and hyperpolarizability for the 14 electron molecules CO and BF. Chemical Physics Letters, 1997, 280, 203-211.	2.6	18
78	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
79	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
80	Hydrogen atoms in the diamond vacancy defect. A quantum mechanical vibrational analysis. Carbon, 2018, 129, 349-356.	10.3	18
81	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
82	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
83	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
84	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
85	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
86	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
87	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
88	Coupled Perturbed Hartree-Fock Calculation of the Static Polarizability for Periodic Systems: Implementation in the CRYSTAL Code. AIP Conference Proceedings, 2007, , .	0.4	13
89	Brillouin Spectroscopy, Calculated Elastic and Bond Properties of GaAsO₄. Inorganic Chemistry, 2010, 49, 9470-9478.	4.0	13
90	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

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91	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
92	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
93	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
94	Long-range coefficients for the low-lying electronic states of LiB. Chemical Physics Letters, 1996, 257, 409-413.	2.6	11
95	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
96	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
97	BiVO3 : A Bi-based material with promising uv-visible light absorption properties. Physical Review B, 2017, 96, .	3.2	11
98	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
99	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
100	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
101	Compton profiles of the isoelectronic BeO and BN molecules: an ab initio study. Chemical Physics Letters, 1996, 263, 767-774.	2.6	10
102	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
103	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
104	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
105	The electronic structure of MgO nanotubes. An ab initio quantum mechanical investigation. Physical Chemistry Chemical Physics, 2013, 15, 13296.	2.8	10
106	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
107	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
108	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

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109	Gauge-dependent ket calculation of the magnetic properties of molecules. Computational and Theoretical Chemistry, 1987, 151, 39-60.	1.5	8
110	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
111	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
112	Long-range coefficients for the low-lying electronic states of BeLi and Be2. Journal of Chemical Physics, 1999, 110, 2051-2058.	3.0	8
113	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
114	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
115	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
116	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
117	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
118	Gauge-dependent ket calculations of dynamical polarizabilities of small molecules. Method and application to H2O. Computational and Theoretical Chemistry, 1988, 166, 97-102.	1.5	7
119	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
120	Ab initiocalculations of the dispersion contribution to the physisorption potential: Application to theN2-BN system. Physical Review B, 2006, 73, .	3.2	7
121	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
122	First-principles calculations of nonlinear optical susceptibility of inorganic materials. Journal of Physics Condensed Matter, 2001, 13, 343-351.	1.8	6
123	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
124	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
125	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
126	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

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127	Topological complexity of potential surfaces and application to C2H2 molecule. Theoretica Chimica Acta, 1994, 88, 285-298.	0.8	5
128	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
129	Computational analysis of strain-induced electronic and optical properties of Zn3As2. Journal of Materials Science, 2020, 55, 5099-5110.	3.7	5
130	Ab initio CI 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
131	Equivariant Morse theory of theN-body problem: Application to potential surfaces in chemistry. Theoretica Chimica Acta, 1993, 86, 297-313.	0.8	4
132	A quantum-mechanical calculation of the dynamic structure factors of magnesium difluoride. International Journal of Quantum Chemistry, 1998, 58, 419-429.	2.0	4
133	Theoretical determination of the ionization cross-section of water. Computational and Theoretical Chemistry, 2002, 577, 17-33.	1.5	4
134	Prediction of electronic (hyper)polarizabilities of titania nanotubes: A DFT periodic study. Computational Materials Science, 2013, 68, 280-286.	3.0	4
135	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
136	Gauge-dependent ket calculation of the magnetic properties of molecules. Computational and Theoretical Chemistry, 1988, 164, 121-134.	1.5	3
137	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
138	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
139	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
140	From anisotropy of dielectric tensors to birefringence: a quantum mechanics approach. Rendiconti Lincei, 2020, 31, 835-851.	2.2	3
141	Rovibronic corrections, temperature and electric field dependence of polarizabilities in LiH and CO. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1990, 87, 989-1000.	0.2	3
142	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
143	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
144	LCAO-LDA calculation of Compton profiles in hexagonal BN; comparison with experiments. Journal of Physics Condensed Matter, 1996, 8, 10425-10434.	1.8	2

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145	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
146	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
147	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
148	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
149	Polarizability and charge density distribution in crystalline urea. AIP Conference Proceedings, 2012, , .	0.4	1
150	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
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