Alessandro Erba

List of Publications by Year
in descending order

98 papers	5,209 citations	147801 31 h-index	88630 70 g-index
101 all docs	101 docs citations	101 times ranked	4784 citing authors

#	Article	IF	Citations
1	Desmarais etÂal. Reply:. Physical Review Letters, 2022, 128, 099702.	7.8	0
2	Spin current density functional theory of Weyl semimetals. Physical Review B, 2022, 105, .	3.2	10
3	Anharmonic Coupling of Stretching Vibrations in Ice: A Periodic VSCF and VCI Description. Journal of Chemical Theory and Computation, 2022, 18, 4428-4437.	5.3	10
4	Charge Density Analysis of Actinide Compounds from the Quantum Theory of Atoms in Molecules and Crystals. Journal of Physical Chemistry Letters, 2021, 12, 1862-1868.	4.6	11
5	Spinâ€“orbit coupling from a two-component self-consistent approach. II. Non-collinear density functional theories. Journal of Chemical Physics, 2021, 154, 204110.	3.0	15
6	Mechanisms for Pressure-Induced Isostructural Phase Transitions in EuO. Physical Review Letters, 2021, 126, 196404.	7.8	7
7	Topology of the Electron Density and of Its Laplacian from Periodic LCAO Calculations on f-Electron Materials: The Case of Cesium Uranyl Chloride. Molecules, 2021, 26, 4227.	3.8	5
8	Perturbation Theory Treatment of Spinâ€“Orbit Coupling, Part I: Double Perturbation Theory Based on a Single-Reference Initial Approximation. Journal of Chemical Theory and Computation, 2021, 17, 4697-4711.	5.3	4
9	Perturbation Theory Treatment of Spinâ€“Orbit Coupling II: A Coupled Perturbed Kohnâ€“Sham Method. Journal of Chemical Theory and Computation, 2021, 17, 4712-4732.	5.3	7
10	Ab initio compressibility of metastable low albite: revealing a lambda-type singularity at pressures of the Earthâ€™s upper mantle. Physics and Chemistry of Minerals, 2020, 47, 1.	0.8	3
11	Thermoelasticity in organic semiconductors determined with terahertz spectroscopy and quantum quasi-harmonic simulations. Journal of Materials Chemistry C, 2020, 8, 10917-10925.	5.5	20
12	Inelastic Neutron Scattering Investigation of MgCl₂ Nanoparticle-Based Zieglerâ€“Natta Catalysts for Olefin Polymerization. ACS Applied Nano Materials, 2020, 3, 11118-11128.	5.0	5
13	Thermoelasticity of Flexible Organic Crystals from Quasi-harmonic Lattice Dynamics: The Case of Copper(II) Acetylacetonate. Journal of Physical Chemistry Letters, 2020, 11, 8543-8548.	4.6	15
14	Adiabatic connection in spin-current density functional theory. Physical Review B, 2020, 102, .	3.2	16
15	Spin-orbit coupling in periodic systems with broken time-reversal symmetry: Formal and computational aspects. Physical Review B, 2020, 101, .	3.2	24
16	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
17	Spin-orbit coupling from a two-component self-consistent approach. II. Non-collinear density functional theories. Journal of Chemical Physics, 2019, 151, 074108.	3.0	5
18	Spin-orbit coupling from a two-component self-consistent approach. I. Generalized Hartree-Fock theory. Journal of Chemical Physics, 2019, 151, 074107.	3.0	20

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19	Fundamental Role of Fock Exchange in Relativistic Density Functional Theory. Journal of Physical Chemistry Letters, 2019, 10, 3580-3585.	4.6	17
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	Quasiâ€Harmonic Lattice Dynamics of a Prototypical Metalâ€“Organic Framework. Advanced Theory and Simulations, 2019, 2, 1900093.	2.8	21
23	Elucidating the structure and dynamics of CO ad-layers on MgO surfaces. Physical Chemistry Chemical Physics, 2019, 21, 26279-26283.	2.8	10
24	Negative thermal expansion of Cu2O studied by quasi-harmonic approximation and cubic force-constant method. Journal of Chemical Physics, 2019, 151, 184109.	3.0	8
25	Thermo-Elasticity of Materials from Quasi-Harmonic Calculations. Minerals (Basel, Switzerland), 2019, 9, 16.	2.0	23
26	Pressure-driven mechanical anisotropy and destabilization in zeolitic imidazolate frameworks. Physical Review B, 2019, 99, .	3.2	27
27	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
28	Generalization of the periodic LCAO approach in the CRYSTAL code to g-type orbitals. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	31
29	Quantumâ€mechanical condensed matter simulations with CRYSTAL. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1360.	14.6	1,277
30	Probing the Mechanochemistry of Metalâ€“Organic Frameworks with Low-Frequency Vibrational Spectroscopy. Journal of Physical Chemistry C, 2018, 122, 27442-27450.	3.1	37
31	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
32	A quantum-mechanical investigation of oxygen vacancies and copper doping in the orthorhombic CaSnO₃ perovskite. Physical Chemistry Chemical Physics, 2018, 20, 20970-20980.	2.8	10
33	Spin localization, magnetic ordering, and electronic properties of strongly correlated <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ln</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:mrow></mml:math> sesquioxides (Ln=La, Ce, Pr, Nd). Physical Review B, 2018, 97, .	3.2	36
34	Intermolecular anharmonicity in molecular crystals: interplay between experimental low-frequency dynamics and quantum quasi-harmonic simulations of solid purine. Chemical Communications, 2017, 53, 3781-3784.	4.1	64
35	Self-consistent hybrid functionals for solids: a fully-automated implementation. Journal of Physics Condensed Matter, 2017, 29, 314001.	1.8	23
36	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

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37	Quantification of cationâ€“anion interactions in crystalline monopotassium and monosodium glutamate salts. Physical Chemistry Chemical Physics, 2017, 19, 28647-28652.	2.8	6
38	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
39	The VN₃H defect in diamond: a quantum-mechanical characterization. Physical Chemistry Chemical Physics, 2017, 19, 22221-22229.	2.8	20
40	Electromechanical Properties of Ba_(1â€“x)Sr_xTiO₃ Perovskite Solid Solutions from First-Principles Calculations. Journal of Physical Chemistry A, 2017, 121, 9409-9414.	2.5	11
41	Anharmonic terahertz dynamics characterisec with first-principles simulations. , 2017, , .		0
42	Piezo-optic and elasto-optic properties of monoclinic triglycine sulfate crystals. Applied Optics, 2017, 56, 9484.	1.8	5
43	Piezooptic coefficients and acoustooptic efficiency of TGS crystals. Ukrainian Journal of Physical Optics, 2017, 18, 46.	13.0	4
44	The internal-strain tensor of crystals for nuclear-relaxed elastic and piezoelectric constants: on the full exploitation of its symmetry features. Physical Chemistry Chemical Physics, 2016, 18, 13984-13992.	2.8	11
45	Piezo-optic and elasto-optic effects in lead molibdate crystals. Optical Materials, 2016, 62, 632-638.	3.6	13
46	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
47	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
48	Thermal properties of molecular crystals through dispersion-corrected quasi-harmonic ab initio calculations: the case of urea. Chemical Communications, 2016, 52, 1820-1823.	4.1	65
49	Piezoelectricity of Functionalized Graphene: A Quantum-Mechanical Rationalization. Journal of Physical Chemistry C, 2016, 120, 7795-7803.	3.1	26
50	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
51	Thermal properties of the orthorhombic CaSnO3 perovskite under pressure from ab initio quasi-harmonic calculations. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	22
52	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
53	Quasi-harmonic treatment of thermal effects on electron charge and momentum densities of solids from ab initio calculations. Acta Crystallographica Section A: Foundations and Advances, 2016, 72, s84-s84.	0.1	0
54	Anharmonic Thermal Oscillations of the Electron Momentum Distribution in Lithium Fluoride. Physical Review Letters, 2015, 115, 117402.	7.8	30

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55	Piezo-optic tensor of crystals from quantum-mechanical calculations. Journal of Chemical Physics, 2015, 143, 144504.	3.0	23
56	Electron density analysis of large (molecular and periodic) systems: A parallel implementation. Journal of Computational Chemistry, 2015, 36, n/a-n/a.	3.3	30
57	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
58	Katoite under pressure: an ab initio investigation of its structural, elastic and vibrational properties sheds light on the phase transition. Physical Chemistry Chemical Physics, 2015, 17, 2660-2669.	2.8	16
59	In silico infrared and Raman spectroscopy under pressure: The case of CaSnO3 perovskite. Journal of Chemical Physics, 2015, 142, 014505.	3.0	28
60	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
61	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
62	Origins of contrasting copper coordination geometries in crystalline copper sulfate pentahydrate. Physical Chemistry Chemical Physics, 2015, 17, 31023-31029.	2.8	34
63	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
64	Hydrogrossular, Ca₃Al₂(SiO₄)_{3â€“x}(H₄O₄)_x: An ab initio investigation of its structural and energetic properties. American Mineralogist, 2015, 100, 2637-2649.	1.9	16
65	Quantum mechanical predictions to elucidate the anisotropic elastic properties of zeolitic imidazolate frameworks: ZIF-4 vs. ZIF-zni. CrystEngComm, 2015, 17, 375-382.	2.6	95
66	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
67	On combining temperature and pressure effects on structural properties of crystals with standard ab initio techniques. Journal of Chemical Physics, 2014, 141, 124115.	3.0	68
68	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
69	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
70	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
71	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
72	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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73	Elasticity of grossularâ€“andradite solid solution: an ab initio investigation. Physical Chemistry Chemical Physics, 2014, 16, 15331.	2.8	16
74	Raman spectrum of NaAlSi₂O₆ jadeite. A quantum mechanical simulation. Journal of Raman Spectroscopy, 2014, 45, 703-709.	2.5	41
75	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
76	Photoelasticity of crystals from theoretical simulations. Physical Review B, 2013, 88, .	3.2	41
77	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
78	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
79	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
80	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
81	Beryllium Oxide Nanotubes and their Connection to the Flat Monolayer. Journal of Physical Chemistry C, 2013, 117, 12864-12872.	3.1	60
82	The vibrational spectrum of CaCO3 aragonite: A combined experimental and quantum-mechanical investigation. Journal of Chemical Physics, 2013, 138, 014201.	3.0	92
83	Anisotropic displacement parameters for molecular crystals from periodic Hartreeâ€“Fock and density functional theory calculations. Acta Crystallographica Section A: Foundations and Advances, 2013, 69, 309-321.	0.3	49
84	Nuclear motion effects on the density matrix of crystals: An ab initio Monte Carlo harmonic approach. Journal of Chemical Physics, 2012, 137, 044114.	3.0	7
85	Cryscor: a program for the post-Hartreeâ€“Fock treatment of periodic systems. Physical Chemistry Chemical Physics, 2012, 14, 7615.	2.8	122
86	Beyond Wigner's theorems: The role of symmetry equivalences in quantum systems. International Journal of Quantum Chemistry, 2012, 112, 3543-3551.	2.0	3
87	Evaluation of the electron momentum density of crystalline systems from ab initio linear combination of atomic orbitals calculations. Journal of Computational Chemistry, 2012, 33, 822-831.	3.3	13
88	Evidence of instantaneous electron correlation from Compton profiles of crystalline silicon. Physical Chemistry Chemical Physics, 2011, 13, 933-936.	2.8	24
89	Electron Densities and Related Properties from the ab-initio Simulation of Crystalline Solids. , 2011, , 79-132.		3
90	Pressure-induced transitions in solid nitrogen: Role of dispersive interactions. Physical Review B, 2011, 84, .	3.2	32

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91	Beyond a single-determinantal description of the density matrix of periodic systems: Experimental versus theoretical Compton profiles of crystalline silicon. Physical Review B, 2011, 83, .	3.2	26
92	Anisotropy of the electron momentum distribution in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-quartz investigated by Compton scattering andab initiosimulations. Physical Review B, 2011, 84, .	3.2	19
93	A post-Hartreeâ€“Fock study of pressure-induced phase transitions in solid nitrogen: The case of the Î±, Î³, and Îµ low-pressure phases. Journal of Chemical Physics, 2011, 134, 074502.	3.0	24
94	A fundamental connection between symmetry and spatial localization properties of basis sets. Theoretical Chemistry Accounts, 2010, 126, 165-175.	1.4	8
95	MP2 versus density-functional theory study of the Compton profiles of crystalline urea. Physical Review B, 2010, 81, .	3.2	43
96	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
97	A local-MP2 approach to the ab initio study of electron correlation in crystals and to the simulation of vibrational spectra: the case of Ice XI. Theoretical Chemistry Accounts, 2009, 123, 327-335.	1.4	13
98	DFT and Local-MP2 Periodic Study of the Structure and Stability of Two Proton-Ordered Polymorphs of Ice. Journal of Physical Chemistry B, 2009, 113, 2347-2354.	2.6	36