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	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	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
4	Cryscor: a program for the post-Hartreeâ€“Fock treatment of periodic systems. Physical Chemistry Chemical Physics, 2012, 14, 7615.	2.8	122
5	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
6	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
7	The vibrational spectrum of CaCO3 aragonite: A combined experimental and quantum-mechanical investigation. Journal of Chemical Physics, 2013, 138, 014201.	3.0	92
8	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
9	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
10	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
11	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
12	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
13	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
14	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
15	Beryllium Oxide Nanotubes and their Connection to the Flat Monolayer. Journal of Physical Chemistry C, 2013, 117, 12864-12872.	3.1	60
16	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
17	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
18	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

#	Article	IF	Citations
19	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
20	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
21	MP2 versus density-functional theory study of the Compton profiles of crystalline urea. Physical Review B, 2010, 81, .	3.2	43
22	Photoelasticity of crystals from theoretical simulations. Physical Review B, 2013, 88, .	3.2	41
23	Raman spectrum of NaAlSi₂O₆ jadeite. A quantum mechanical simulation. Journal of Raman Spectroscopy, 2014, 45, 703-709.	2.5	41
24	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
25	Probing the Mechanochemistry of Metalâ€“Organic Frameworks with Low-Frequency Vibrational Spectroscopy. Journal of Physical Chemistry C, 2018, 122, 27442-27450.	3.1	37
26	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
27	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
28	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
29	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:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> sesquioxides (Ln=La, Ce, Pr, Nd). Physical Review B, 2018, 97, .	3.2	36
30	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
31	Origins of contrasting copper coordination geometries in crystalline copper sulfate pentahydrate. Physical Chemistry Chemical Physics, 2015, 17, 31023-31029.	2.8	34
32	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
33	Pressure-induced transitions in solid nitrogen: Role of dispersive interactions. Physical Review B, 2011, 84, .	3.2	32
34	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
35	Generalization of the periodic LCAO approach in the CRYSTAL code to g-type orbitals. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	31
36	Anharmonic Thermal Oscillations of the Electron Momentum Distribution in Lithium Fluoride. Physical Review Letters, 2015, 115, 117402.	7.8	30

#	Article	IF	Citations
37	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
38	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
39	In silico infrared and Raman spectroscopy under pressure: The case of CaSnO3 perovskite. Journal of Chemical Physics, 2015, 142, 014505.	3.0	28
40	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
41	Pressure-driven mechanical anisotropy and destabilization in zeolitic imidazolate frameworks. Physical Review B, 2019, 99, .	3.2	27
42	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
43	Piezoelectricity of Functionalized Graphene: A Quantum-Mechanical Rationalization. Journal of Physical Chemistry C, 2016, 120, 7795-7803.	3.1	26
44	Evidence of instantaneous electron correlation from Compton profiles of crystalline silicon. Physical Chemistry Chemical Physics, 2011, 13, 933-936.	2.8	24
45	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
46	Spin-orbit coupling in periodic systems with broken time-reversal symmetry: Formal and computational aspects. Physical Review B, 2020, 101, .	3.2	24
47	Piezo-optic tensor of crystals from quantum-mechanical calculations. Journal of Chemical Physics, 2015, 143, 144504.	3.0	23
48	Self-consistent hybrid functionals for solids: a fully-automated implementation. Journal of Physics Condensed Matter, 2017, 29, 314001.	1.8	23
49	Thermo-Elasticity of Materials from Quasi-Harmonic Calculations. Minerals (Basel, Switzerland), 2019, 9, 16.	2.0	23
50	Thermal properties of the orthorhombic CaSnO3 perovskite under pressure from ab initio quasi-harmonic calculations. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	22
51	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
52	Quasiâ€Harmonic Lattice Dynamics of a Prototypical Metalâ€“Organic Framework. Advanced Theory and Simulations, 2019, 2, 1900093.	2.8	21
53	The VN₃H defect in diamond: a quantum-mechanical characterization. Physical Chemistry Chemical Physics, 2017, 19, 22221-22229.	2.8	20
54	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

#	Article	IF	Citations
55	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
56	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
57	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
58	Fundamental Role of Fock Exchange in Relativistic Density Functional Theory. Journal of Physical Chemistry Letters, 2019, 10, 3580-3585.	4.6	17
59	Elasticity of grossularâ€“andradite solid solution: an ab initio investigation. Physical Chemistry Chemical Physics, 2014, 16, 15331.	2.8	16
60	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
61	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
62	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
63	Adiabatic connection in spin-current density functional theory. Physical Review B, 2020, 102, .	3.2	16
64	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
65	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
66	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
67	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
68	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
69	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
70	Piezo-optic and elasto-optic effects in lead molibdate crystals. Optical Materials, 2016, 62, 632-638.	3.6	13
71	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
72	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

#	Article	IF	Citations
73	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
74	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
75	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
76	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
77	Elucidating the structure and dynamics of CO ad-layers on MgO surfaces. Physical Chemistry Chemical Physics, 2019, 21, 26279-26283.	2.8	10
78	Spin current density functional theory of Weyl semimetals. Physical Review B, 2022, 105, .	3.2	10
79	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
80	A fundamental connection between symmetry and spatial localization properties of basis sets. Theoretical Chemistry Accounts, 2010, 126, 165-175.	1.4	8
81	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
82	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
83	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
84	Mechanisms for Pressure-Induced Isostructural Phase Transitions in EuO. Physical Review Letters, 2021, 126, 196404.	7.8	7
85	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
86	Quantification of cationâ€–anion interactions in crystalline monopotassium and monosodium glutamate salts. Physical Chemistry Chemical Physics, 2017, 19, 28647-28652.	2.8	6
87	Piezo-optic and elasto-optic properties of monoclinic triglycine sulfate crystals. Applied Optics, 2017, 56, 9484.	1.8	5
88	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
89	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
90	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

#	Article	IF	Citations
91	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
92	Piezooptic coefficients and acoustooptic efficiency of TGS crystals. Ukrainian Journal of Physical Optics, 2017, 18, 46.	13.0	4
93	Electron Densities and Related Properties from the ab-initio Simulation of Crystalline Solids. , 2011, , 79-132.		3
94	Beyond Wigner's theorems: The role of symmetry equivalences in quantum systems. International Journal of Quantum Chemistry, 2012, 112, 3543-3551.	2.0	3
95	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
96	Anharmonic terahertz dynamics characterisec with first-principles simulations. , 2017, , .		0
97	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
98	Desmarais etÂal. Reply:. Physical Review Letters, 2022, 128, 099702.	7.8	0