Bartolomeo Civalleri

List of Publications by Year
in descending order

169 papers	14,529 citations	31976 53 h-index	19749 117 g-index
172 all docs	172 docs citations	172 times ranked	12137 citing authors

#	Article	IF	Citations
1	Disclosing the Complex Structure of UiO-66 Metal Organic Framework: A Synergic Combination of Experiment and Theory. Chemistry of Materials, 2011, 23, 1700-1718.	6.7	1,420
2	Quantumâ€mechanical condensed matter simulations with CRYSTAL. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1360.	14.6	1,277
3	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
4	CRYSTAL: a computational tool for the ab initio study of the electronic properties of crystals. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.8	824
5	The calculation of the vibrational frequencies of crystalline compounds and its implementation in the CRYSTAL code. Journal of Computational Chemistry, 2004, 25, 888-897.	3.3	796
6	B3LYP augmented with an empirical dispersion term (B3LYP-D*) as applied to molecular crystals. CrystEngComm, 2008, 10, 405-410.	2.6	775
7	H₂storage in isostructural UiO-67 and UiO-66 MOFs. Physical Chemistry Chemical Physics, 2012, 14, 1614-1626.	2.8	415
8	Computational and Experimental Studies on the Adsorption of CO, N₂, and CO₂on Mg-MOF-74. Journal of Physical Chemistry C, 2010, 114, 11185-11191.	3.1	307
9	Hartreeâ€“Fock geometry optimisation of periodic systems with the Crystal code. Chemical Physics Letters, 2001, 348, 131-138.	2.6	294
10	Polarization properties of ZnO and BeO:â€ƒAnab initiostudy through the Berry phase and Wannier functions approaches. Physical Review B, 2001, 65, .	3.2	213
11	Exceptionally Low Shear Modulus in a Prototypical Imidazole-Based Metal-Organic Framework. Physical Review Letters, 2012, 108, 095502.	7.8	210
12	Identifying the Role of Terahertz Vibrations in Metal-Organic Frameworks: From Gate-Opening Phenomenon to Shear-Driven Structural Destabilization. Physical Review Letters, 2014, 113, 215502.	7.8	202
13	Ab-initio prediction of materials properties with CRYSTAL: MOF-5 as a case study. CrystEngComm, 2006, 8, 364-371.	2.6	187
14	Ab-initio calculation of elastic constants of crystalline systems with the CRYSTAL code. Computer Physics Communications, 2009, 180, 1753-1759.	7.5	178
15	Effect of Benzoic Acid as a Modulator in the Structure of UiO-66: An Experimental and Computational Study. Journal of Physical Chemistry C, 2017, 121, 9312-9324.	3.1	176
16	Intermolecular Interaction Energies in Molecular Crystals: Comparison and Agreement of Localized MÃ¸llerâ€“Plesset 2, Dispersion-Corrected Density Functional, and Classical Empirical Two-Body Calculations. Journal of Physical Chemistry A, 2011, 115, 11179-11186.	2.5	169
17	Flexibility in a Metalâ€“Organic Framework Material Controlled by Weak Dispersion Forces: The Bistability of MILâ€53(Al). Angewandte Chemie - International Edition, 2010, 49, 7501-7503.	13.8	158
18	Experimental and Quantum Chemical Studies on the Adsorption of Carbon Dioxide on Alkali-Metal-Exchanged ZSM-5 Zeolites. Journal of Physical Chemistry B, 2000, 104, 10978-10988.	2.6	156

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19	Periodic ab initio study of structural and vibrational features of hexagonal hydroxyapatite Ca10(PO4)6(OH)2. Physical Chemistry Chemical Physics, 2006, 8, 2464.	2.8	153
20	The CRYSTAL code, 1976â€“2020 and beyond, a long story. Journal of Chemical Physics, 2020, 152, 204111.	3.0	133
21	Geometrical Correction for the Inter- and Intramolecular Basis Set Superposition Error in Periodic Density Functional Theory Calculations. Journal of Physical Chemistry A, 2013, 117, 9282-9292.	2.5	123
22	Heats of Adsorption of CO and CO₂ in Metalâ€“Organic Frameworks: Quantum Mechanical Study of CPO-27-M (M = Mg, Ni, Zn). Journal of Physical Chemistry C, 2011, 115, 21777-21784.	3.1	122
23	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
24	Ab Initio Quantum Simulation in Solid State Chemistry. Reviews in Computational Chemistry, 2005, , 1-125.	1.5	120
25	Discovering connections between terahertz vibrations and elasticity underpinning the collective dynamics of the HKUST-1 metalâ€“organic framework. CrystEngComm, 2016, 18, 4303-4312.	2.6	96
26	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
27	Ab Initio Investigation of Structure and Cohesive Energy of Crystalline Urea. Journal of Physical Chemistry B, 2007, 111, 26-33.	2.6	87
28	Fundamental Aspects of H₂S Adsorption on CPO-27-Ni. Journal of Physical Chemistry C, 2013, 117, 15615-15622.	3.1	85
29	Assessment of Different Quantum Mechanical Methods for the Prediction of Structure and Cohesive Energy of Molecular Crystals. Journal of Chemical Theory and Computation, 2016, 12, 3340-3352.	5.3	85
30	Cation Selectivity in Alkali-Exchanged Chabazite:Â An ab Initio Periodic Study. Chemistry of Materials, 2003, 15, 3996-4004.	6.7	83
31	Interaction of Glycine with Isolated Hydroxyl Groups at the Silica Surface:â€‰ First Principles B3LYP Periodic Simulation. Langmuir, 2006, 22, 6593-6604.	3.5	83
32	Carbon Dioxide Adsorption in Amineâ€Functionalized Mixedâ€Ligand Metalâ€“Organic Frameworks of UiOâ€66 Topology. ChemSusChem, 2014, 7, 3382-3388.	6.8	83
33	Periodic local MÃllerâ€“Plesset second order perturbation theory method applied to molecular crystals: Study of solid NH3 and CO2 using extended basis sets. Journal of Chemical Physics, 2010, 132, 134706.	3.0	81
34	Structural, Electronic, and Vibrational Properties of the Tiâ€”Oâ€”Ti Quantum Wires in the Titanosilicate ETS-10. Journal of Physical Chemistry B, 2004, 108, 1328-1336.	2.6	79
35	Normal Vibrational Analysis of the Syndiotactic Polystyrene s(2/1)2 Helix. Journal of Physical Chemistry B, 2009, 113, 5059-5071.	2.6	78
36	Prediction Uncertainty of Density Functional Approximations for Properties of Crystals with Cubic Symmetry. Journal of Physical Chemistry A, 2015, 119, 5288-5304.	2.5	78

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37	First Principles Calculations of the Adsorption of NH3on a Periodic Model of the Silica Surface. Journal of Physical Chemistry B, 2000, 104, 9491-9499.	2.6	75
38	Role of dispersive interactions in layered materials: a periodic B3LYP and B3LYP-D* study of Mg(OH)2, Ca(OH)2 and kaolinite. Journal of Materials Chemistry, 2009, 19, 2564.	6.7	75
39	A periodic ab initio study of the structure and relative stability of silica polymorphs. Chemical Physics Letters, 1998, 292, 394-402.	2.6	74
40	Quantum Mechanical ab Initio Characterization of a Simple Periodic Model of the Silica Surface. Journal of Physical Chemistry B, 1999, 103, 2165-2171.	2.6	74
41	A comparison between plane wave and Gaussian-type orbital basis sets for hydrogen bonded systems: Formic acid as a test case. Journal of Chemical Physics, 2007, 127, 154102.	3.0	72
42	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
43	FFSiOH: a New Force Field for Silica Polymorphs and Their Hydroxylated Surfaces Based on Periodic B3LYP Calculations. Chemistry of Materials, 2008, 20, 2522-2531.	6.7	68
44	Structureâ€“activity relationships of simple molecules adsorbed on CPO-27-Ni metalâ€“organic framework: In situ experiments vs. theory. Catalysis Today, 2012, 182, 67-79.	4.4	67
45	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
46	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
47	Metalâ€“Organic Frameworks and Hybrid Materials: From Fundamentals to Applications. CrystEngComm, 2015, 17, 197-198.	2.6	64
48	Role of dispersive interactions in the CO adsorption on MgO(001): periodic B3LYP calculations augmented with an empirical dispersion term. Physical Chemistry Chemical Physics, 2010, 12, 6382.	2.8	60
49	Physisorption of aromatic organic contaminants at the surface of hydrophobic/hydrophilic silica geosorbents: a B3LYP-D modeling study. Physical Chemistry Chemical Physics, 2010, 12, 6357.	2.8	60
50	Detecting Molecular Rotational Dynamics Complementing the Low-Frequency Terahertz Vibrations in a Zirconium-Based Metal-Organic Framework. Physical Review Letters, 2017, 118, 255502.	7.8	60
51	Ab Initio Calculation of the Crystalline Structure and IR Spectrum of Polymers: Nylon 6 Polymorphs. Journal of Physical Chemistry B, 2012, 116, 8299-8311.	2.6	56
52	Ab Initio Study of the Adducts of Small Molecules with the Isolated Hydroxyl of Silica and the BrÃ¸nsted Site in Zeolites:â€‰ A Comparison between B3-LYP and MP2 Methods. Journal of Physical Chemistry B, 1998, 102, 2373-2382.	2.6	55
53	Modeling physisorption with the ONIOM method: the case of NH3 at the isolated hydroxyl group of the silica surface. Chemical Physics Letters, 2001, 341, 625-632.	2.6	54
54	H-Chabazite with variable Si/Al ratio: stability and OH vibrational frequency computed in a periodic LCAO B3-LYP approach. Chemical Physics Letters, 2000, 318, 247-255.	2.6	52

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55	Coupling of framework modes and adsorbate vibrations for CO2 molecularly adsorbed on alkali ZSM-5 zeolites: Mid- and far-infrared spectroscopy andab initiomodeling. Journal of Chemical Physics, 2002, 117, 10274-10282.	3.0	52
56	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, 223-239.	0.8	52
57	Revisiting the identity of Î´-MgCl2: Part I. Structural disorder studied by synchrotron X-ray total scattering. Journal of Catalysis, 2020, 385, 76-86.	6.2	51
58	Thermo-chemical and thermo-physical properties of the high-pressure phase anhydrous B (Mg14Si5O24): An ab-initio all-electron investigation. American Mineralogist, 2010, 95, 563-573.	1.9	50
59	Vibrational modes of isolated hydroxyls of silica computed ab initio in a cluster approach. Chemical Physics Letters, 1998, 294, 103-108.	2.6	49
60	Ab initio study of van der Waals and hydrogen-bonded molecular crystals with a periodic local-MP2 method. CrystEngComm, 2010, 12, 2429.	2.6	49
61	Approaching the theoretical limit in periodic local MP2 calculations with atomic-orbital basis sets: The case of LiH. Journal of Chemical Physics, 2011, 134, 214105.	3.0	49
62	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
63	Interaction of H2with Alkali-Metal-Exchanged Zeolites:â€‰a Quantum Mechanical Study. Journal of Physical Chemistry C, 2007, 111, 2505-2513.	3.1	47
64	Normal Vibrational Analysis of a trans-Planar Syndiotactic Polystyrene Chain. Journal of Physical Chemistry B, 2007, 111, 6327-6335.	2.6	47
65	Neutral vs Zwitterionic Glycine Forms at the Water/Silica Interface: Structure, Energies, and Vibrational Features from B3LYP Periodic Simulations. Langmuir, 2008, 24, 14027-14034.	3.5	47
66	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
67	Isoreticular zirconium-based metalâ€“organic frameworks: discovering mechanical trends and elastic anomalies controlling chemical structure stability. Physical Chemistry Chemical Physics, 2016, 18, 9079-9087.	2.8	46
68	Hydrogarnet defect in chabazite and sodalite zeolites: A periodic Hartreeâ€“Fock and B3-LYP study. Journal of Chemical Physics, 2002, 117, 5337-5346.	3.0	44
69	Thermophysical properties of the Î±â€“Î²â€“Î³ polymorphs of Mg2SiO4: a computational study. Physics and Chemistry of Minerals, 2009, 36, 87-106.	0.8	44
70	A quantum-mechanical study of the vinyl fluoride adsorbed on the rutile TiO2(110) surface. Surface Science, 2006, 600, 305-317.	1.9	43
71	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
72	Elucidating the Drug Release from Metalâ€“Organic Framework Nanocomposites via In Situ Synchrotron Microspectroscopy and Theoretical Modeling. ACS Applied Materials & Interfaces, 2020, 12, 5147-5156.	8.0	43

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73	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
74	Structure and Energetics of SiO2Polymorphs by Quantum-Mechanical and Semiclassical Approaches. Journal of Physical Chemistry B, 2000, 104, 7259-7265.	2.6	40
75	Probing Dielectric Properties of Metalâ€“Organic Frameworks: MIL-53(Al) as a Model System for Theoretical Predictions and Experimental Measurements via Synchrotron Far- and Mid-Infrared Spectroscopy. Journal of Physical Chemistry Letters, 2017, 8, 5035-5040.	4.6	39
76	On choosing the best density functional approximation. Chemical Modelling, 0, , 168-185.	0.4	38
77	Understanding and Controlling the Dielectric Response of Metalâ€“Organic Frameworks. ChemPlusChem, 2018, 83, 308-316.	2.8	36
78	Density functional study of hydrogen-bonded systems: Energetic and vibrational features of some gas-phase adducts of hydrogen fluoride. Computational and Theoretical Chemistry, 1997, 419, 227-238.	1.5	35
79	Flexibility in a Metalâ€“Organic Framework Material Controlled by Weak Dispersion Forces: The Bistability of MILâ€53(Al). Angewandte Chemie, 2010, 122, 7663-7665.	2.0	35
80	Periodic B3LYP study of hydroxyapatite (001) surface modelled by thin layer slabs. European Journal of Mineralogy, 2007, 19, 757-767.	1.3	34
81	Theoretical Study of Molecular Hydrogen Adsorption in Mg-Exchanged Chabazite. Journal of Physical Chemistry C, 2007, 111, 1871-1873.	3.1	34
82	Communication: A combined periodic density functional and incremental wave-function-based approach for the dispersion-accounting time-resolved dynamics of 4He nanodroplets on surfaces: 4He/graphene. Journal of Chemical Physics, 2014, 141, 151102.	3.0	34
83	Thermodynamic modelling of Mg(BH4)2. Journal of Alloys and Compounds, 2015, 645, S64-S68.	5.5	34
84	Cage-like clusters as models for the hydroxyls of silica: ab initio calculation of 1H and 29Si NMR chemical shifts. Chemical Physics Letters, 1999, 299, 443-450.	2.6	33
85	Uniplanar Orientations as a Tool To Assign Vibrational Modes of Polymer Chain. Macromolecules, 2007, 40, 3895-3897.	4.8	33
86	Carbon monoxide adsorption on alkali and proton-exchanged chabazite: anab-initioperiodic study using the CRYSTAL code. Molecular Physics, 2005, 103, 2559-2571.	1.7	32
87	An ab initio parameterized interatomic force field for hydroxyapatite. Journal of Materials Chemistry, 2007, 17, 2061.	6.7	32
88	A computational multiscale strategy to the study of amorphous materials. Theoretical Chemistry Accounts, 2007, 117, 933-942.	1.4	32
89	IR spectroscopy of crystalline polymers from ab initio calculations: Nylon 6,6. Vibrational Spectroscopy, 2013, 66, 83-92.	2.2	32
90	Periodic B3-LYP calculations on H-Edingtonites, both alone and interacting with acetylene. Physical Chemistry Chemical Physics, 1999, 1, 545-553.	2.8	31

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91	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
92	Dielectric Properties of Zeolitic Imidazolate Frameworks in the Broad-Band Infrared Regime. Journal of Physical Chemistry Letters, 2018, 9, 2678-2684.	4.6	31
93	Thermo-chemical and thermo-physical properties of stishovite: An ab-initio all-electron investigation. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2009, 33, 457-468.	1.6	27
94	Theoretical and experimental study on Mg(BH4)2â€“Zn(BH4)2 mixed borohydrides. Journal of Alloys and Compounds, 2013, 580, S282-S286.	5.5	27
95	Stability vs. reactivity: understanding the adsorption properties of Ni3(BTP)2 by experimental and computational methods. Dalton Transactions, 2013, 42, 6450.	3.3	27
96	Assessment of Density Functional Approximations for Highly Correlated Oxides: The Case of CeO₂ and Ce₂O₃. Journal of Chemical Theory and Computation, 2018, 14, 4914-4927.	5.3	27
97	Electron-density and electrostatic-potential features of orthorhombic chlorine trifluoride. Mendeleev Communications, 2010, 20, 161-164.	1.6	26
98	Defect Engineering in Metalâ€“Organic Framework Nanocrystals: Implications for Mechanical Properties and Performance. ACS Applied Nano Materials, 2022, 5, 6398-6409.	5.0	26
99	Cagelike Clusters as Models for the Isolated Hydroxyls of Silica:ÂAb InitioB3-LYP Calculations of the Interaction with Ammoniaâ€. Langmuir, 1999, 15, 5829-5835.	3.5	25
100	Revisiting the identity of Î´-MgCl2: Part II. Morphology and exposed surfaces studied by vibrational spectroscopies and DFT calculation. Journal of Catalysis, 2020, 387, 1-11.	6.2	25
101	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
102	Double-hybrid density-functional theory applied to molecular crystals. Journal of Chemical Physics, 2014, 141, 044105.	3.0	24
103	Benchmarking dispersion and geometrical counterpoise corrections for costâ€effective largeâ€scale DFT calculations of water adsorption on graphene. Journal of Computational Chemistry, 2014, 35, 1789-1800.	3.3	24
104	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
105	Structural, electronic, and vibrational properties of solid Sr(OH)2, calculated with different Hamiltonians. Journal of Chemical Physics, 2003, 119, 1045-1052.	3.0	23
106	An Ab Initio Periodic Study of Acidic Chabazite as a Candidate for Dihydrogen Storage. Journal of Physical Chemistry B, 2006, 110, 10467-10474.	2.6	23
107	Hydrophobic Behavior of Dehydroxylated Silica Surfaces: A B3LYP Periodic Study. Journal of Physical Chemistry C, 2010, 114, 19984-19992.	3.1	23
108	Periodic density functional theory calculations for 3-dimensional polyacetylene with empirical dispersion terms. Physical Chemistry Chemical Physics, 2010, 12, 3289.	2.8	23

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109	Oxalyl dihydrazide polymorphism: a periodic dispersion-corrected DFT and MP2 investigation. CrystEngComm, 2014, 16, 102-109.	2.6	23
110	Range-separated double-hybrid density-functional theory applied to periodic systems. Journal of Chemical Physics, 2015, 143, 102811.	3.0	21
111	Extending and assessing composite electronic structure methods to the solid state. Journal of Chemical Physics, 2019, 151, 121101.	3.0	21
112	Quasiâ€Harmonic Lattice Dynamics of a Prototypical Metalâ€“Organic Framework. Advanced Theory and Simulations, 2019, 2, 1900093.	2.8	21
113	A review of the computational studies of proton- and metal-exchanged chabazites as media for molecular hydrogen storage performed with the CRYSTAL code. International Journal of Hydrogen Energy, 2008, 33, 746-754.	7.1	20
114	Hydrogen storage of Mgâ€“Zn mixed metal borohydrides. Journal of Alloys and Compounds, 2014, 615, S702-S705.	5.5	20
115	Tunable Fluorescein-Encapsulated Zeolitic Imidazolate Framework-8 Nanoparticles for Solid-State Lighting. ACS Applied Nano Materials, 2021, 4, 10321-10333.	5.0	20
116	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
117	Application of Metal-Organic Frameworks and Covalent Organic Frameworks as (Photo)Active Material in Hybrid Photovoltaic Technologies. Energies, 2020, 13, 5602.	3.1	19
118	Hydrogen atoms in the diamond vacancy defect. A quantum mechanical vibrational analysis. Carbon, 2018, 129, 349-356.	10.3	18
119	Structural and Optical Properties of Struvite. Elucidating Structure of Infrared Spectrum in High Frequency Range. Journal of Physical Chemistry A, 2020, 124, 8668-8678.	2.5	18
120	Gaussian Basis Sets for Crystalline Solids: All-Purpose Basis Set Libraries vs System-Specific Optimizations. Journal of Chemical Theory and Computation, 2020, 16, 2192-2201.	5.3	18
121	17O-EPR determination of the structure and dynamics of copper single-metal sites in zeolites. Nature Communications, 2021, 12, 4638.	12.8	18
122	Theoretical and experimental characterization of pyrazolato-based Ni(ii) metalâ€“organic frameworks. Journal of Materials Chemistry, 2012, 22, 22592.	6.7	17
123	Cost-Effective Quantum Mechanical Approach for Predicting Thermodynamic and Mechanical Stability of Pure-Silica Zeolites. ACS Omega, 2019, 4, 1838-1846.	3.5	17
124	Low energy excitations in NiO based on a direct Î”-SCF approach. Journal of Physics Condensed Matter, 2018, 30, 495901.	1.8	16
125	CRYSPLOT: A new tool to visualize physical and chemical properties of molecules, polymers, surfaces, and crystalline solids. Journal of Computational Chemistry, 2019, 40, 2329-2338.	3.3	16
126	Testing the combination of Hartreeâ€“Fock exchange and Wilsonâ€“Levy correlation for weakly bonded extended systems. Chemical Physics Letters, 2008, 451, 287-292.	2.6	15

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127	Elucidating the Interaction of CO2 in the Giant Metalâ€“Organic Framework MIL-100 through Large-Scale Periodic Ab Initio Modeling. Journal of Physical Chemistry C, 2019, 123, 28677-28687.	3.1	15
128	Repulsive and attractive interactions between Brnsted sites and hydrocarbon species with partial carbocationic character in restricted spaces: comparison of IR results and ab initiocalculations. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 3893-3898.	1.7	14
129	HCl and HClâˆ™Base Adducts in Silicalite Channels as Models of Acidâˆ™Base Interactions in Zeolites:Â An IR and Theoretical Study. Journal of Physical Chemistry B, 1998, 102, 10753-10764.	2.6	14
130	The katoite hydrogarnet Si-free Ca3Al2([OH]4)3: A periodic Hartreeâ€“Fock and B3-LYP study. Journal of Chemical Physics, 2004, 121, 1005-1013.	3.0	14
131	Raman and infrared vibrational frequencies and elastic properties of solid BaFCl calculated with various Hamiltonians: anab initiostudy. Journal of Physics Condensed Matter, 2005, 17, 535-548.	1.8	14
132	Impact of Pressure and Temperature on the Broadband Dielectric Response of the HKUST-1 Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2019, 123, 29427-29435.	3.1	14
133	Spectroscopic and thermodynamic study of the H-bonding of olefins onto the isolated hydroxyl of amorphous silica. Physical Chemistry Chemical Physics, 1999, 1, 4649-4654.	2.8	13
134	(CD3CN)2H+ adducts in anhydrous H3PW12O40: a FTIR study. Physical Chemistry Chemical Physics, 2001, 3, 1345-1347.	2.8	13
135	The Interpretation of the Short Range Disorder in the Fluorene-TCNE Crystal Structure. International Journal of Molecular Sciences, 2004, 5, 93-100.	4.1	13
136	Entrapping Molecules in Zeolites Nanocavities: A Thermodynamic and Ab-Initio Study. Origins of Life and Evolution of Biospheres, 2004, 34, 69-77.	1.9	13
137	Hydroxylated crystalline edingtonite silica faces as models for the amorphous silica surface. Journal of Physics: Conference Series, 2008, 117, 012026.	0.4	13
138	Comment on â€œAccurate Hartree-Fock energy of extended systems using large Gaussian basis setsâ€• Physical Review B, 2010, 81, .	3.2	13
139	Cost-effective composite methods for large-scale solid-state calculations. Faraday Discussions, 2020, 224, 292-308.	3.2	13
140	Investigation on the Decomposition Enthalpy of Novel Mixed Mg_(1â€“x)Zn_x(BH₄)₂ Borohydrides by Means of Periodic DFT Calculations. Journal of Physical Chemistry C, 2014, 118, 23468-23475.	3.1	12
141	The Structure of Monomeric Hydroxo-Cu^{II} Species in Cu-CHA. A Quantitative Assessment. Journal of the American Chemical Society, 2022, 144, 13079-13083.	13.7	12
142	Ab initio periodic study of the conformational behavior of glycine helical homopeptides. Journal of Computational Chemistry, 2010, 31, 1777-1784.	3.3	11
143	Adducts of alkali-metal ions with the Cî€‡C triple bond: an experimental and ab initio study. Physical Chemistry Chemical Physics, 2002, 4, 1658-1664.	2.8	10
144	Metalâ€“Organic Frameworks in Italy: From synthesis and advanced characterization to theoretical modeling and applications. Coordination Chemistry Reviews, 2021, 437, 213861.	18.8	10

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145	Metalâ€“organic frameworks properties from hybrid density functional approximations. Journal of Chemical Physics, 2022, 156, 094706.	3.0	10
146	H3SiOH and F3SiOH as models for isolated hydroxyl groups of amorphous silica: an ab initio study of the adducts with dihydrogen and carbon monoxide. Surface Science, 1998, 412-413, 141-157.	1.9	9
147	New ultrasoft pseudopotentials for the study of silicates. Molecular Simulation, 2002, 28, 213-237.	2.0	9
148	Acid Strength of Low-Valence Dopant Ions in Microporous Zeolites and AlPOs. Journal of Physical Chemistry B, 2003, 107, 11866-11870.	2.6	9
149	The unique Raman fingerprint of boron nitride substitution patterns in graphene. Physical Chemistry Chemical Physics, 2016, 18, 20270-20275.	2.8	9
150	Interfacing CRYSTAL/AMBER to Optimize QM/MM Lennardâ€“Jones Parameters for Water and to Study Solvation of TiO2 Nanoparticles. Molecules, 2018, 23, 2958.	3.8	9
151	Ab-initio thermal physics and Cr-isotopic fractionation of MgCr2O4. American Mineralogist, 2007, 92, 98-108.	1.9	8
152	Ab initio modeling of layered materials with the CRYSTAL code: an overview. Zeitschrift FÃ¼r Kristallographie, 2009, 224, 241-250.	1.1	8
153	Combined study of structural properties on metal-organic frameworks with same topology but different linkers or metal. Journal of Physics: Conference Series, 2013, 430, 012134.	0.4	8
154	Implicit Solvation Using a Generalized Finite-Difference Approach in CRYSTAL: Implementation and Results for Molecules, Polymers, and Surfaces. Journal of Chemical Theory and Computation, 2018, 14, 5969-5983.	5.3	8
155	On the Use of Benchmarks for Multiple Properties. Computation, 2016, 4, 20.	2.0	7
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