# Bartolomeo Civalleri

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | Metalâ€“organic frameworks properties from hybrid density functional approximations. Journal of Chemical Physics, 2022, 156, 094706. | 3.0 | 10 |
| 2 | Desmarais etÂal. Reply:. Physical Review Letters, 2022, 128, 099702. | 7.8 | 0 |
| 3 | Defect Engineering in Metalâ€“Organic Framework Nanocrystals: Implications for Mechanical Properties and Performance. ACS Applied Nano Materials, 2022, 5, 6398-6409. | 5.0 | 26 |
| 4 | The Structure of Monomeric Hydroxo-Cu<sup>II</sup> Species in Cu-CHA. A Quantitative Assessment. Journal of the American Chemical Society, 2022, 144, 13079-13083. | 13.7 | 12 |
| 5 | Simulation of nanosizing effects in the decomposition of Ca(BH4)2 through atomistic thin film models. Research on Chemical Intermediates, 2021, 47, 345-356. | 2.7 | 7 |
| 6 | Mechanisms for Pressure-Induced Isostructural Phase Transitions in EuO. Physical Review Letters, 2021, 126, 196404. | 7.8 | 7 |
| 7 | Metalâ€“Organic Frameworks in Italy: From synthesis and advanced characterization to theoretical modeling and applications. Coordination Chemistry Reviews, 2021, 437, 213861. | 18.8 | 10 |
| 8 | 17O-EPR determination of the structure and dynamics of copper single-metal sites in zeolites. Nature Communications, 2021, 12, 4638. | 12.8 | 18 |
| 9 | Tunable Fluorescein-Encapsulated Zeolitic Imidazolate Framework-8 Nanoparticles for Solid-State Lighting. ACS Applied Nano Materials, 2021, 4, 10321-10333. | 5.0 | 20 |
| 10 | 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 |
| 11 | 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 |
| 12 | Cost-effective composite methods for large-scale solid-state calculations. Faraday Discussions, 2020, 224, 292-308. | 3.2 | 13 |
| 13 | Challenges for large scale simulation: general discussion. Faraday Discussions, 2020, 224, 309-332. | 3.2 | 2 |
| 14 | Inelastic Neutron Scattering Investigation of MgCl<sub>2</sub> Nanoparticle-Based Zieglerâ€“Natta Catalysts for Olefin Polymerization. ACS Applied Nano Materials, 2020, 3, 11118-11128. | 5.0 | 5 |
| 15 | Application of Metal-Organic Frameworks and Covalent Organic Frameworks as (Photo)Active Material in Hybrid Photovoltaic Technologies. Energies, 2020, 13, 5602. | 3.1 | 19 |
| 16 | The CRYSTAL code, 1976â€“2020 and beyond, a long story. Journal of Chemical Physics, 2020, 152, 204111. | 3.0 | 133 |
| 17 | Analytical calculation of the solventâ€accessible surface area and its nuclear gradients by stereographic projection: A general approach for molecules, polymers, nanotubes, helices, and surfaces. Journal of Computational Chemistry, 2020, 41, 1464-1479. | 3.3 | 7 |
| 18 | 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 |

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| 19 | 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 |
| 20 | 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 |
| 21 | 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 |
| 22 | Cost-Effective Quantum Mechanical Approach for Predicting Thermodynamic and Mechanical Stability of Pure-Silica Zeolites. ACS Omega, 2019, 4, 1838-1846. | 3.5 | 17 |
| 23 | 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 |
| 24 | Extending and assessing composite electronic structure methods to the solid state. Journal of Chemical Physics, 2019, 151, 121101. | 3.0 | 21 |
| 25 | Quasiâ€Harmonic Lattice Dynamics of a Prototypical Metalâ€“Organic Framework. Advanced Theory and Simulations, 2019, 2, 1900093. | 2.8 | 21 |
| 26 | Frontiers in Modeling Metalâ€“Organic Frameworks. Advanced Theory and Simulations, 2019, 2, 1900196. | 2.8 | 3 |
| 27 | 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 |
| 28 | Understanding and Controlling the Dielectric Response of Metalâ€“Organic Frameworks. ChemPlusChem, 2018, 83, 308-316. | 2.8 | 36 |
| 29 | Quantumâ€mechanical condensed matter simulations with CRYSTAL. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1360. | 14.6 | 1,277 |
| 30 | 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 |
| 31 | Dielectric Properties of Zeolitic Imidazolate Frameworks in the Broad-Band Infrared Regime. Journal of Physical Chemistry Letters, 2018, 9, 2678-2684. | 4.6 | 31 |
| 32 | Hydrogen atoms in the diamond vacancy defect. A quantum mechanical vibrational analysis. Carbon, 2018, 129, 349-356. | 10.3 | 18 |
| 33 | 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 |
| 34 | Low energy excitations in NiO based on a direct Î”-SCF approach. Journal of Physics Condensed Matter, 2018, 30, 495901. | 1.8 | 16 |
| 35 | 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 |
| 36 | Assessment of Density Functional Approximations for Highly Correlated Oxides: The Case of CeO<sub>2</sub> and Ce<sub>2</sub>O<sub>3</sub>. Journal of Chemical Theory and Computation, 2018, 14, 4914-4927. | 5.3 | 27 |

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| 37 | Topical collection of papers collected on the occasion of the XLI congress of the theoretical chemists of Latin expression (CHITEL 2015 - Torino - Italy). Theoretical Chemistry Accounts, 2017, 136, 1. | 1.4 | 0 |
| 38 | 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 |
| 39 | Exploring the Linear Optical Properties of Borazine (B<sub>3</sub>N<sub>3</sub>) Doped Graphenes. 0D Flakes vs 2D Sheets. Journal of Physical Chemistry C, 2017, 121, 709-722. | 3.1 | 24 |
| 40 | 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 |
| 41 | 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 |
| 42 | On the Use of Benchmarks for Multiple Properties. Computation, 2016, 4, 20. | 2.0 | 7 |
| 43 | The unique Raman fingerprint of boron nitride substitution patterns in graphene. Physical Chemistry Chemical Physics, 2016, 18, 20270-20275. | 2.8 | 9 |
| 44 | 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 |
| 45 | 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 |
| 46 | 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 |
| 47 | 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 |
| 48 | 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 |
| 49 | Range-separated double-hybrid density-functional theory applied to periodic systems. Journal of Chemical Physics, 2015, 143, 102811. | 3.0 | 21 |
| 50 | 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 |
| 51 | Thermodynamic modelling of Mg(BH4)2. Journal of Alloys and Compounds, 2015, 645, S64-S68. | 5.5 | 34 |
| 52 | Metalâ€“Organic Frameworks and Hybrid Materials: From Fundamentals to Applications. CrystEngComm, 2015, 17, 197-198. | 2.6 | 64 |
| 53 | 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 |
| 54 | 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 |

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| 55 | Double-hybrid density-functional theory applied to molecular crystals. Journal of Chemical Physics, 2014, 141, 044105. | 3.0 | 24 |
| 56 | 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 |
| 57 | Hydrogen storage of Mgâ€“Zn mixed metal borohydrides. Journal of Alloys and Compounds, 2014, 615, S702-S705. | 5.5 | 20 |
| 58 | 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 |
| 59 | Oxalyl dihydrazide polymorphism: a periodic dispersion-corrected DFT and MP2 investigation. CrystEngComm, 2014, 16, 102-109. | 2.6 | 23 |
| 60 | 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 |
| 61 | Carbon Dioxide Adsorption in Amineâ€Functionalized Mixedâ€Ligand Metalâ€“Organic Frameworks of UiOâ€66 Topology. ChemSusChem, 2014, 7, 3382-3388. | 6.8 | 83 |
| 62 | Investigation on the Decomposition Enthalpy of Novel Mixed Mg<sub>(1â€“x)</sub>Zn<sub>x</sub>(BH<sub>4</sub>)<sub>2</sub> Borohydrides by Means of Periodic DFT Calculations. Journal of Physical Chemistry C, 2014, 118, 23468-23475. | 3.1 | 12 |
| 63 | Fundamental Aspects of H<sub>2</sub>S Adsorption on CPO-27-Ni. Journal of Physical Chemistry C, 2013, 117, 15615-15622. | 3.1 | 85 |
| 64 | 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 |
| 65 | 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 |
| 66 | IR spectroscopy of crystalline polymers from ab initio calculations: Nylon 6,6. Vibrational Spectroscopy, 2013, 66, 83-92. | 2.2 | 32 |
| 67 | Stability vs. reactivity: understanding the adsorption properties of Ni3(BTP)2 by experimental and computational methods. Dalton Transactions, 2013, 42, 6450. | 3.3 | 27 |
| 68 | 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 |
| 69 | 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 |
| 70 | Exceptionally Low Shear Modulus in a Prototypical Imidazole-Based Metal-Organic Framework. Physical Review Letters, 2012, 108, 095502. | 7.8 | 210 |
| 71 | Polarizability and charge density distribution in crystalline urea. AIP Conference Proceedings, 2012, , . | 0.4 | 1 |
| 72 | Theoretical and experimental characterization of pyrazolato-based Ni(ii) metalâ€“organic frameworks. Journal of Materials Chemistry, 2012, 22, 22592. | 6.7 | 17 |

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| 73 | 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 |
| 74 | H<sub>2</sub>storage in isostructural UiO-67 and UiO-66 MOFs. Physical Chemistry Chemical Physics, 2012, 14, 1614-1626. | 2.8 | 415 |
| 75 | 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 |
| 76 | 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 |
| 77 | Heats of Adsorption of CO and CO<sub>2</sub> 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 |
| 78 | 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 |
| 79 | 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 |
| 80 | 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 |
| 81 | Ab-Initio Fully Periodic Characterization of MOF-74-M (M = Mg, Mn, Ni, Zn): Structures and Enthalpies of Adsorption. Materials Research Society Symposia Proceedings, 2011, 1366, 1. | 0.1 | 0 |
| 82 | Ab initio periodic study of the conformational behavior of glycine helical homopeptides. Journal of Computational Chemistry, 2010, 31, 1777-1784. | 3.3 | 11 |
| 83 | 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 |
| 84 | 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 |
| 85 | Electron-density and electrostatic-potential features of orthorhombic chlorine trifluoride. Mendeleev Communications, 2010, 20, 161-164. | 1.6 | 26 |
| 86 | 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 |
| 87 | Performance of 12 DFT functionals in the study of crystal systems: Al<sub>2</sub>SiO<sub>5</sub> orthosilicates and Al hydroxides as a case study. International Journal of Quantum Chemistry, 2010, 110, 2260-2273. | 2.0 | 42 |
| 88 | Magnetic interactions in Ca<sub>3</sub>Fe<sub>2</sub>Ge<sub>3</sub>O<sub>12</sub> and Ca<sub>3</sub>Cr<sub>2</sub>Ge<sub>3</sub>O<sub>12</sub> garnets. An ab initio allâ€electron quantum mechanical simulation. International Journal of Quantum Chemistry, 2010, 110, 2192-2201. | 2.0 | 6 |
| 89 | Periodic local MÃ¸llerâ€“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 |
| 90 | 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 |

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| 91 | Hydrophobic Behavior of Dehydroxylated Silica Surfaces: A B3LYP Periodic Study. Journal of Physical Chemistry C, 2010, 114, 19984-19992. | 3.1 | 23 |
| 92 | Comment on â€œAccurate Hartree-Fock energy of extended systems using large Gaussian basis setsâ€• Physical Review B, 2010, 81, . | 3.2 | 13 |
| 93 | Computational and Experimental Studies on the Adsorption of CO, N<sub>2</sub>, and CO<sub>2</sub>on Mg-MOF-74. Journal of Physical Chemistry C, 2010, 114, 11185-11191. | 3.1 | 307 |
| 94 | Periodic density functional theory calculations for 3-dimensional polyacetylene with empirical dispersion terms. Physical Chemistry Chemical Physics, 2010, 12, 3289. | 2.8 | 23 |
| 95 | 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 |
| 96 | 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 |
| 97 | 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 |
| 98 | 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 |
| 99 | Ab initio modeling of layered materials with the CRYSTAL code: an overview. Zeitschrift FÃ¼r Kristallographie, 2009, 224, 241-250. | 1.1 | 8 |
| 100 | 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 |
| 101 | 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 |
| 102 | Ab-initio calculation of elastic constants of crystalline systems with the CRYSTAL code. Computer Physics Communications, 2009, 180, 1753-1759. | 7.5 | 178 |
| 103 | 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 |
| 104 | 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 |
| 105 | Normal Vibrational Analysis of the Syndiotactic Polystyrene s(2/1)2 Helix. Journal of Physical Chemistry B, 2009, 113, 5059-5071. | 2.6 | 78 |
| 106 | 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 |
| 107 | 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 |
| 108 | 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 |

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| 109 | Hydroxylated crystalline edingtonite silica faces as models for the amorphous silica surface. Journal of Physics: Conference Series, 2008, 117, 012026. | 0.4 | 13 |
| 110 | B3LYP augmented with an empirical dispersion term (B3LYP-D*) as applied to molecular crystals. CrystEngComm, 2008, 10, 405-410. | 2.6 | 775 |
| 111 | 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 |
| 112 | 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 |
| 113 | Ab Initioinvestigation of the interaction of H<sub>2</sub>with lithium exchanged low-silica chabazites. Journal of Physics: Conference Series, 2008, 117, 012012. | 0.4 | 3 |
| 114 | Periodic B3LYP study of hydroxyapatite (001) surface modelled by thin layer slabs. European Journal of Mineralogy, 2007, 19, 757-767. | 1.3 | 34 |
| 115 | Ab-initio thermal physics and Cr-isotopic fractionation of MgCr2O4. American Mineralogist, 2007, 92, 98-108. | 1.9 | 8 |
| 116 | An ab initio parameterized interatomic force field for hydroxyapatite. Journal of Materials Chemistry, 2007, 17, 2061. | 6.7 | 32 |
| 117 | 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 |
| 118 | Uniplanar Orientations as a Tool To Assign Vibrational Modes of Polymer Chain. Macromolecules, 2007, 40, 3895-3897. | 4.8 | 33 |
| 119 | Interaction of H2with Alkali-Metal-Exchanged Zeolites:â€‰ a Quantum Mechanical Study. Journal of Physical Chemistry C, 2007, 111, 2505-2513. | 3.1 | 47 |
| 120 | Normal Vibrational Analysis of a trans-Planar Syndiotactic Polystyrene Chain. Journal of Physical Chemistry B, 2007, 111, 6327-6335. | 2.6 | 47 |
| 121 | Theoretical Study of Molecular Hydrogen Adsorption in Mg-Exchanged Chabazite. Journal of Physical Chemistry C, 2007, 111, 1871-1873. | 3.1 | 34 |
| 122 | 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 |
| 123 | Ab Initio Investigation of Structure and Cohesive Energy of Crystalline Urea. Journal of Physical Chemistry B, 2007, 111, 26-33. | 2.6 | 87 |
| 124 | A computational multiscale strategy to the study of amorphous materials. Theoretical Chemistry Accounts, 2007, 117, 933-942. | 1.4 | 32 |
| 125 | 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 |
| 126 | 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 |

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| 127 | 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 |
| 128 | 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 |
| 129 | Ab-initio prediction of materials properties with CRYSTAL: MOF-5 as a case study. CrystEngComm, 2006, 8, 364-371. | 2.6 | 187 |
| 130 | A quantum-mechanical study of the vinyl fluoride adsorbed on the rutile TiO2(110) surface. Surface Science, 2006, 600, 305-317. | 1.9 | 43 |
| 131 | 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 |
| 132 | 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 |
| 133 | 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 |
| 134 | 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 |
| 135 | Ab Initio Quantum Simulation in Solid State Chemistry. Reviews in Computational Chemistry, 2005, , 1-125. | 1.5 | 120 |
| 136 | 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 |
| 137 | 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 |
| 138 | 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 |
| 139 | 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 |
| 140 | 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 |
| 141 | Cation Selectivity in Alkali-Exchanged Chabazite:Â An ab Initio Periodic Study. Chemistry of Materials, 2003, 15, 3996-4004. | 6.7 | 83 |
| 142 | Acid Strength of Low-Valence Dopant Ions in Microporous Zeolites and AlPOs. Journal of Physical Chemistry B, 2003, 107, 11866-11870. | 2.6 | 9 |
| 143 | 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 |
| 144 | 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 |

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| 145 | New ultrasoft pseudopotentials for the study of silicates. Molecular Simulation, 2002, 28, 213-237. | 2.0 | 9 |
| 146 | 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 |
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