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List of Publications by Year
in descending order

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63	795	471509	580821
papers	citations	17 h-index	25 g-index

63	63	63	460
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The vibrational features of hydroxylapatite and type A carbonated apatite: A first principle contribution. American Mineralogist, 2013, 98, 752-759.	1.9	55
2	Comparison between Gaussian-type orbitals and plane wave ab initio density functional theory modeling of layer silicates: Talc [Mg3Si4O10(OH)2] as model system. Journal of Chemical Physics, 2013, 139, 204101.	3.0	44
3	Periodic ab initio bulk investigation of hydroxylapatite and type A carbonated apatite with both pseudopotential and all-electron basis sets for calcium atoms. American Mineralogist, 2013, 98, 410-416.	1.9	35
4	DFT investigation of structural and vibrational properties of type B and mixed A-B carbonated hydroxylapatite. American Mineralogist, 2014, 99, 117-127.	1.9	35
5	Raman spectroscopic investigation on the molecular structure of apatite and collagen in osteoporotic cortical bone. Journal of the Mechanical Behavior of Biomedical Materials, 2017, 65, 264-273.	3.1	35
6	The compressional behaviour and the mechanical properties of talc [Mg3Si4O10(OH)2]: a density functional theory investigation. Physics and Chemistry of Minerals, 2014, 41, 639-650.	0.8	34
7	Density functional investigation of the thermo-physical and thermo-chemical properties of 2M1 muscovite. American Mineralogist, 2015, 100, 935-944.	1.9	34
8	Density functional investigation of the thermophysical and thermochemical properties of talc [Mg3Si4O10(OH)2]. Physics and Chemistry of Minerals, 2015, 42, 151-162.	0.8	31
9	Nanoscale cross-correlated AFM, Kelvin probe, elastic modulus and quantum mechanics investigation of clay mineral surfaces: The case of chlorite. Applied Clay Science, 2016, 131, 175-181.	5.2	30
10	Structural, vibrational and thermophysical properties of pyrophyllite by semi-empirical density functional modelling. Physics and Chemistry of Minerals, 2015, 42, 609-627.	0.8	27
11	Effects of fluorine content on the elastic behavior of topaz [Al₂SiO₄(F,OH)₂]. American Mineralogist, 2017, 102, 347-356.	1.9	27
12	First-principles study of structural and surface properties of (001) and (010) surfaces of hydroxylapatite and carbonated hydroxylapatite. Journal of Applied Crystallography, 2016, 49, 1893-1903.	4.5	22
13	First principle investigation of the mechanical properties of natural layered nanocomposite: Clinochlore as a model system for heterodesmic structures. Composite Structures, 2018, 202, 551-558.	5.8	22
14	Single Molecule Investigation of Glycineâ€“Chlorite Interaction by Cross-Correlated Scanning Probe Microscopy and Quantum Mechanics Simulations. Langmuir, 2015, 31, 4453-4463.	3.5	21
15	CO<sub>3</sup>2â€“</sup> Mobility in Carbonate Apatite As Revealed by Density Functional Modeling. Journal of Physical Chemistry C, 2014, 118, 1364-1369.	3.1	20
16	Secondâ€order elastic constants of hexagonal hydroxylapatite (P6₃) from ab initio quantum mechanics: Comparison between DFT functionals and basis sets. International Journal of Quantum Chemistry, 2018, 118, e25500.	2.0	19
17	Effect of mechanical stress on the Raman and infrared bands of hydroxylapatite: A quantum mechanical first principle investigation. Journal of the Mechanical Behavior of Biomedical Materials, 2018, 77, 683-692.	3.1	17
18	Nucleotides, RNA and DNA selective adsorption on atomic-flat Mgâ€“Al-hydroxysilicate substrates. Micro and Nano Letters, 2011, 6, 922.	1.3	16

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19	Equation of state and second-order elastic constants of portlandite Ca(OH)2 and brucite Mg(OH)2. Physics and Chemistry of Minerals, 2019, 46, 101-117.	0.8	16
20	Benchmarking dispersion-corrected DFT methods for the evaluation of materials with anisotropic properties: structural, electronic, dielectric, optical and vibrational analysis of calcite (CaCO₃, space group R3l„c). Physical Chemistry Chemical Physics, 2021, 23, 18899-18907.	2.8	16
21	Equation of state of hexagonal hydroxylapatite (P6₃) as obtained from density functional theory simulations. International Journal of Quantum Chemistry, 2018, 118, e25553.	2.0	15
22	Hydroxylapatite and Related Minerals in Bone and Dental Tissues: Structural, Spectroscopic and Mechanical Properties from a Computational Perspective. Biomolecules, 2021, 11, 728.	4.0	15
23	Amino acids-clay interaction at the nano-atomic scale: The l-alanine-chlorite system. Applied Clay Science, 2019, 172, 28-39.	5.2	13
24	Infrared and Raman spectroscopic features of clinochlore Mg6Si4O10(OH)8: A density functional theory contribution. Applied Clay Science, 2020, 197, 105779.	5.2	13
25	Thermomechanical, electronic and thermodynamic properties of ZnS cubic polymorphs: anab initioinvestigation on the zinc-blendeâ€“rock-salt phase transition. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 1042-1059.	1.1	12
26	Electronic and optical properties of graphene/molybdenite bilayer composite. Composite Structures, 2021, 255, 112978.	5.8	12
27	3D meso-nanostructures in cleaved and nanolithographed Mg-Al-hydroxysilicate (clinochlore): Topology, crystal-chemistry, and surface properties. Applied Clay Science, 2019, 169, 74-80.	5.2	11
28	Probing the interaction of (001) carbonated hydroxylapatite surfaces with water: a density functional investigation. Micro and Nano Letters, 2018, 13, 4-8.	1.3	11
29	Effects of dehydration and grinding on the mechanical shear behaviour of Ca-rich montmorillonite. Applied Clay Science, 2018, 152, 239-248.	5.2	10
30	First principle investigation of the thermomechanical properties of type A carbonated apatite. International Journal of Quantum Chemistry, 2020, 120, e26069.	2.0	8
31	Monte Carlo SEM-EDS micro- and nanoanalysis of ultrathin gold leaves in glass mosaic tesserae: Thickness effects and measurement strategy. Measurement: Journal of the International Measurement Confederation, 2018, 129, 211-217.	5.0	7
32	Thermodynamic and thermoelastic properties of wurtzite-ZnS by density functional theory. American Mineralogist, 2020, 105, 1212-1222.	1.9	7
33	Nanoâ€atomic scale hydrophobic/philic confinement of peptides on mineral surfaces by crossâ€correlated SPM and quantum mechanical DFT analysis. Journal of Microscopy, 2020, 280, 204-221.	1.8	7
34	Thermodynamic, elastic, and vibrational (IR/Raman) behavior of mixed type-AB carbonated hydroxylapatite by density functional theory. American Mineralogist, 2021, 106, 1928-1939.	1.9	7
35	DFT Simulation of the Water Molecule Interaction with the (00l) Surface of Montmorillonite. Minerals (Basel, Switzerland), 2021, 11, 501.	2.0	7
36	Monte Carlo simulation of the effect of shape and thickness on SEM-EDS microanalysis of asbestos fibres and bundles: the case of anthophyllite, tremolite and actinolite. IOP Conference Series: Materials Science and Engineering, 2018, 304, 012019.	0.6	6

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37	Water adsorption behaviour on (001) pyrophyllite surface from ab initio Density Functional Theory simulations. Applied Clay Science, 2021, 212, 106221.	5.2	6
38	Scanning probe microscopy with vertically oriented cantilevers made easy. Measurement Science and Technology, 2012, 23, 085903.	2.6	5
39	Nanoscale oligopeptide adsorption behaviour on chlorite as revealed by scanning probe microscopy and density functional simulations. Applied Clay Science, 2020, 197, 105777.	5.2	5
40	Interaction at the nanoscale of fundamental biological molecules with minerals. Advances in Nano Research, 2013, 1, 133-151.	0.9	5
41	Mineral surfaceâ€“organic matter interactions: basics and applications. IOP Conference Series: Materials Science and Engineering, 2012, 32, 012027.	0.6	4
42	SEM-EDS nanoanalysis of mineral composite materials: A Monte Carlo approach. Composite Structures, 2021, 259, 113227.	5.8	4
43	Elastic properties of heterodesmic composite structures: The case of calcite CaCO3 (space group) Tj ETQq1 1 0.784314 rgBT /Overlock Part C: Open Access, 2021, 6, 100184.	3.2	4
44	Interaction of organic molecules with layer silicates, oxides and hydroxides and related surface-nano-characterization techniques. , 2011, , 313-334.		4
45	Thermal, X-ray Diffraction and Oedometric Analyses of Silt-Waste/NaOH-Activated Metakaolin Geopolymer Composite. Journal of Composites Science, 2021, 5, 269.	3.0	4
46	Study of the variation of the optical properties of calcite with applied stress, useful for specific rock and material mechanics. Scientific Reports, 2022, 12, 299.	3.3	4
47	Dataset on the piezo-spectroscopic behaviour of hydroxylapatite: Effect of mechanical stress on the Raman and Infrared vibrational bands from ab initio quantum mechanical simulations. Data in Brief, 2018, 18, 325-333.	1.0	3
48	Crystal-chemical and structural data related to the equation of state and second-order elastic constants of portlandite Ca(OH)2 and brucite Mg(OH)2. Data in Brief, 2018, 21, 2367-2375.	1.0	3
49	Ceramic Recipes: Cross-correlated analytical strategy for the characterization of the Iron Age pottery from ancient Karkemish (Turkey). Measurement: Journal of the International Measurement Confederation, 2018, 128, 180-188.	5.0	3
50	Monte Carlo SEM-EDS Nano-Microanalysis Strategy of Historical Mineral Pigments: The Simulation of the Egyptian Blue from Pompeii (Italy) as an Example. Minerals (Basel, Switzerland), 2020, 10, 807.	2.0	3
51	Thermodynamic and thermoelastic data of georesources raw minerals: Zinc sulphide and apatite. Data in Brief, 2020, 29, 105265.	1.0	3
52	Development of A Nano-Apatite Based Composite Sealer for Endodontic Root Canal Filling. Journal of Composites Science, 2021, 5, 30.	3.0	3
53	QUANTAS: a Python software for the analysis of thermodynamics and elastic behavior of solids fromab initioquantum mechanical simulations and experimental data. Journal of Applied Crystallography, 2022, 55, 386-396.	4.5	3
54	Structural and elastic behaviour of aragonite at high-pressure: A contribution from first-principle simulations. Computational Materials Science, 2022, 212, 111600.	3.0	3

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55	Anisotropy and directional elastic behavior data obtained from the second-order elastic constants of portlandite Ca(OH)2 and brucite Mg(OH)2. Data in Brief, 2018, 21, 1375-1380.	1.0	2
56	Nanomorphological investigation of graphite surface after cryoâ€ultrasonication in liquid nitrogen by atomic force microscopy. Micro and Nano Letters, 2018, 13, 546-551.	1.3	2
57	Simulated infrared and Raman spectroscopy, complex dielectric function and refractive index dataset of monoclinic C2/m stoichiometric clinochlore Mg6Si4O10(OH)8 as obtained from Density Functional Theory. Data in Brief, 2020, 32, 106208.	1.0	1
58	Mineral diagnostics: SEM-EDS Monte Carlo strategy for optimised measurements of ultrathin fragments in Cultural Heritage studies. Acta IMEKO (2012), 2021, 10, 193.	0.7	1
59	In Vivo Effects of Two In-Office Vital Tooth Bleaching Systems on Enamel Permeability. Journal of Composites Science, 2021, 5, 98.	3.0	1
60	Fibre-Reinforced Geopolymer Composites Micro-Nanochemistry by SEM-EDS Simulations. Journal of Composites Science, 2021, 5, 214.	3.0	1
61	Monte Carlo strategy for SEM-EDS micro-nanoanalysis of geopolymer composites. Composites Part C: Open Access, 2021, 6, 100183.	3.2	1
62	Scanning probe â€“ atomic force microscopy: new developments and applications. IOP Conference Series: Materials Science and Engineering, 2014, 55, 012019.	0.6	0
63	In Vitro Comparison of Root Surface Treatment Effect between Root Scaling with Ultrasonic Inserts and Gracey Curette and Polishing with Different Cleaning Pastes. Applied Sciences (Switzerland), 2021, 11, 5967.	2.5	0