Giovanni Valdre'

List of Publications by Year
in descending order

57	931	394421	526287
papers	citations	19 h-index	27 g-index

57	57	57	593
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	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
3	Structural and elastic behaviour of aragonite at high-pressure: A contribution from first-principle simulations. Computational Materials Science, 2022, 212, 111600.	3.0	3
4	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
5	Development of A Nano-Apatite Based Composite Sealer for Endodontic Root Canal Filling. Journal of Composites Science, 2021, 5, 30.	3.0	3
6	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
7	DFT Simulation of the Water Molecule Interaction with the (00l) Surface of Montmorillonite. Minerals (Basel, Switzerland), 2021, 11, 501.	2.0	7
8	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
9	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
10	Fibre-Reinforced Geopolymer Composites Micro-Nanochemistry by SEM-EDS Simulations. Journal of Composites Science, 2021, 5, 214.	3.0	1
11	Thermally Treated Waste Silt as Filler in Geopolymer Cement. Materials, 2021, 14, 5102.	2.9	6
12	Water adsorption behaviour on (001) pyrophyllite surface from ab initio Density Functional Theory simulations. Applied Clay Science, 2021, 212, 106221.	5.2	6
13	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
14	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
15	First principle investigation of the thermomechanical properties of type A carbonated apatite. International Journal of Quantum Chemistry, 2020, 120, e26069.	2.0	8
16	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
17	Thermodynamic and thermoelastic properties of wurtzite-ZnS by density functional theory. American Mineralogist, 2020, 105, 1212-1222.	1.9	7
18	Preface to StSPM2019EV special issue. Journal of Microscopy, 2020, 280, 181-182.	1.8	0

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19	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
20	Thermodynamic and thermoelastic data of georesources raw minerals: Zinc sulphide and apatite. Data in Brief, 2020, 29, 105265.	1.0	3
21	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
22	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
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	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
25	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
26	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
27	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
28	Effects of dehydration and grinding on the mechanical shear behaviour of Ca-rich montmorillonite. Applied Clay Science, 2018, 152, 239-248.	5.2	10
29	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
30	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
31	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
32	Effects of fluorine content on the elastic behavior of topaz [Al₂SiO₄(F,OH)₂]. American Mineralogist, 2017, 102, 347-356.	1.9	27
33	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
34	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
35	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
36	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

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37	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
38	Elastic behaviour and phase stability of pyrophyllite and talc at high pressure and temperature. Physics and Chemistry of Minerals, 2015, 42, 309-318.	0.8	11
39	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
40	Density functional investigation of the thermo-physical and thermo-chemical properties of 2M1 muscovite. American Mineralogist, 2015, 100, 935-944.	1.9	34
41	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
42	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
43	CO₃^{2â€“} Mobility in Carbonate Apatite As Revealed by Density Functional Modeling. Journal of Physical Chemistry C, 2014, 118, 1364-1369.	3.1	20
44	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
45	On the crystal structure and compressional behavior of talc: a mineral of interest in petrology and material science. Physics and Chemistry of Minerals, 2013, 40, 145-156.	0.8	32
46	The vibrational features of hydroxylapatite and type A carbonated apatite: A first principle contribution. American Mineralogist, 2013, 98, 752-759.	1.9	55
47	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
48	Interaction at the nanoscale of fundamental biological molecules with minerals. Advances in Nano Research, 2013, 1, 133-151.	0.9	5
49	SPM nanolithography of hydroxy-silicates. Nanotechnology, 2012, 23, 385301.	2.6	13
50	Mineral surfaceâ€“organic matter interactions: basics and applications. IOP Conference Series: Materials Science and Engineering, 2012, 32, 012027.	0.6	4
51	The role of microstrain on the thermostructural behaviour of industrial kaolin deformed by ball milling at low mechanical load. International Journal of Mineral Processing, 2012, 102-103, 69-77.	2.6	29
52	Zeolitic-type Bronsted-Lowry sites distribution imaged on clinochlore. American Mineralogist, 2011, 96, 1461-1466.	1.9	16
53	Crystallographic features and cleavage nanomorphology of chlinochlore: Specific applications. Clays and Clay Minerals, 2009, 57, 183-193.	1.3	16
54	Natural nanoscale surface potential of clinochlore and its ability to align nucleotides and drive DNA conformational change. European Journal of Mineralogy, 2007, 19, 309-319.	1.3	19

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55	High spatial resolution PEELS characterization of FeAl nanograins prepared by mechanical alloying. Acta Materialia, 1999, 47, 2303-2311.	7.9	21
56	Importance of microanalysis in understanding mechanism of transformation in active glassy biomaterials. , 1996, 31, 475-480.		26
57	Diffusion-weighted spatial information from1H relaxation in restricted geometries. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1992, 14, 745-759.	0.4	27