

Giovanni Valdre'

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	The vibrational features of hydroxylapatite and type A carbonated apatite: A first principle contribution. <i>American Mineralogist</i> , 2013, 98, 752-759.	1.9	55
2	Comparison between Gaussian-type orbitals and plane wave <i>ab initio</i> density functional theory modeling of layer silicates: Talc [Mg ₃ Si ₄ O ₁₀ (OH) ₂] as model system. <i>Journal of Chemical Physics</i> , 2013, 139, 204101.	3.0	44
3	Periodic <i>ab initio</i> bulk investigation of hydroxylapatite and type A carbonated apatite with both pseudopotential and all-electron basis sets for calcium atoms. <i>American Mineralogist</i> , 2013, 98, 410-416.	1.9	35
4	DFT investigation of structural and vibrational properties of type B and mixed A-B carbonated hydroxylapatite. <i>American Mineralogist</i> , 2014, 99, 117-127.	1.9	35
5	Raman spectroscopic investigation on the molecular structure of apatite and collagen in osteoporotic cortical bone. <i>Journal of the Mechanical Behavior of Biomedical Materials</i> , 2017, 65, 264-273.	3.1	35
6	The compressional behaviour and the mechanical properties of talc [Mg ₃ Si ₄ O ₁₀ (OH) ₂]: a density functional theory investigation. <i>Physics and Chemistry of Minerals</i> , 2014, 41, 639-650.	0.8	34
7	Density functional investigation of the thermo-physical and thermo-chemical properties of 2M1 muscovite. <i>American Mineralogist</i> , 2015, 100, 935-944.	1.9	34
8	On the crystal structure and compressional behavior of talc: a mineral of interest in petrology and material science. <i>Physics and Chemistry of Minerals</i> , 2013, 40, 145-156.	0.8	32
9	Density functional investigation of the thermophysical and thermochemical properties of talc [Mg ₃ Si ₄ O ₁₀ (OH) ₂]. <i>Physics and Chemistry of Minerals</i> , 2015, 42, 151-162.	0.8	31
10	Nanoscale cross-correlated AFM, Kelvin probe, elastic modulus and quantum mechanics investigation of clay mineral surfaces: The case of chlorite. <i>Applied Clay Science</i> , 2016, 131, 175-181.	5.2	30
11	The role of microstrain on the thermostructural behaviour of industrial kaolin deformed by ball milling at low mechanical load. <i>International Journal of Mineral Processing</i> , 2012, 102-103, 69-77.	2.6	29
12	Diffusion-weighted spatial information from 1H relaxation in restricted geometries. <i>Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics</i> , 1992, 14, 745-759.	0.4	27
13	Structural, vibrational and thermophysical properties of pyrophyllite by semi-empirical density functional modelling. <i>Physics and Chemistry of Minerals</i> , 2015, 42, 609-627.	0.8	27
14	Effects of fluorine content on the elastic behavior of topaz [Al ₂ Si ₄ (F,OH) ₂]. <i>American Mineralogist</i> , 2017, 102, 347-356.	1.9	27
15	Importance of microanalysis in understanding mechanism of transformation in active glassy biomaterials. , 1996, 31, 475-480.		26
16	First-principles study of structural and surface properties of (001) and (010) surfaces of hydroxylapatite and carbonated hydroxylapatite. <i>Journal of Applied Crystallography</i> , 2016, 49, 1893-1903.	4.5	22
17	First principle investigation of the mechanical properties of natural layered nanocomposite: Clinocllore as a model system for heterodesmic structures. <i>Composite Structures</i> , 2018, 202, 551-558.	5.8	22
18	High spatial resolution PEELS characterization of FeAl nanograins prepared by mechanical alloying. <i>Acta Materialia</i> , 1999, 47, 2303-2311.	7.9	21

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19	Single Molecule Investigation of Glycine-Chlorite Interaction by Cross-Correlated Scanning Probe Microscopy and Quantum Mechanics Simulations. <i>Langmuir</i> , 2015, 31, 4453-4463.	3.5	21
20	CO ₃ ²⁻ Mobility in Carbonate Apatite As Revealed by Density Functional Modeling. <i>Journal of Physical Chemistry C</i> , 2014, 118, 1364-1369.	3.1	20
21	Natural nanoscale surface potential of clinocllore and its ability to align nucleotides and drive DNA conformational change. <i>European Journal of Mineralogy</i> , 2007, 19, 309-319.	1.3	19
22	Second-order elastic constants of hexagonal hydroxylapatite (P6 ₃) from <i>ab initio</i> quantum mechanics: Comparison between DFT functionals and basis sets. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25500.	2.0	19
23	Effect of mechanical stress on the Raman and infrared bands of hydroxylapatite: A quantum mechanical first principle investigation. <i>Journal of the Mechanical Behavior of Biomedical Materials</i> , 2018, 77, 683-692.	3.1	17
24	Crystallographic features and cleavage nanomorphology of clinocllore: Specific applications. <i>Clays and Clay Minerals</i> , 2009, 57, 183-193.	1.3	16
25	Zeolitic-type Bronsted-Lowry sites distribution imaged on clinocllore. <i>American Mineralogist</i> , 2011, 96, 1461-1466.	1.9	16
26	Equation of state and second-order elastic constants of portlandite Ca(OH) ₂ and brucite Mg(OH) ₂ . <i>Physics and Chemistry of Minerals</i> , 2019, 46, 101-117.	0.8	16
27	Benchmarking dispersion-corrected DFT methods for the evaluation of materials with anisotropic properties: structural, electronic, dielectric, optical and vibrational analysis of calcite (CaCO ₃ , space group <i>R</i> _{3c}). <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18899-18907.	2.8	16
28	Equation of state of hexagonal hydroxylapatite (P6 ₃) as obtained from density functional theory simulations. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25553.	2.0	15
29	Hydroxylapatite and Related Minerals in Bone and Dental Tissues: Structural, Spectroscopic and Mechanical Properties from a Computational Perspective. <i>Biomolecules</i> , 2021, 11, 728.	4.0	15
30	SPM nanolithography of hydroxy-silicates. <i>Nanotechnology</i> , 2012, 23, 385301.	2.6	13
31	Amino acids-clay interaction at the nano-atomic scale: The l-alanine-chlorite system. <i>Applied Clay Science</i> , 2019, 172, 28-39.	5.2	13
32	Thermomechanical, electronic and thermodynamic properties of ZnS cubic polymorphs: an <i>ab initio</i> investigation on the zinc-blende-rock-salt phase transition. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2019, 75, 1042-1059.	1.1	12
33	Elastic behaviour and phase stability of pyrophyllite and talc at high pressure and temperature. <i>Physics and Chemistry of Minerals</i> , 2015, 42, 309-318.	0.8	11
34	3D meso-nanostructures in cleaved and nanolithographed Mg-Al-hydroxysilicate (clinocllore): Topology, crystal-chemistry, and surface properties. <i>Applied Clay Science</i> , 2019, 169, 74-80.	5.2	11
35	Probing the interaction of (001) carbonated hydroxylapatite surfaces with water: a density functional investigation. <i>Micro and Nano Letters</i> , 2018, 13, 4-8.	1.3	11
36	Effects of dehydration and grinding on the mechanical shear behaviour of Ca-rich montmorillonite. <i>Applied Clay Science</i> , 2018, 152, 239-248.	5.2	10

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37	First principle investigation of the thermomechanical properties of type A carbonated apatite. International Journal of Quantum Chemistry, 2020, 120, e26069.	2.0	8
38	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
39	Thermodynamic and thermoelastic properties of wurtzite-ZnS by density functional theory. American Mineralogist, 2020, 105, 1212-1222.	1.9	7
40	Nanoatomic scale hydrophobic/philic confinement of peptides on mineral surfaces by cross-correlated SPM and quantum mechanical DFT analysis. Journal of Microscopy, 2020, 280, 204-221.	1.8	7
41	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
42	DFT Simulation of the Water Molecule Interaction with the (001) Surface of Montmorillonite. Minerals (Basel, Switzerland), 2021, 11, 501.	2.0	7
43	Thermally Treated Waste Silt as Filler in Geopolymer Cement. Materials, 2021, 14, 5102.	2.9	6
44	Water adsorption behaviour on (001) pyrophyllite surface from ab initio Density Functional Theory simulations. Applied Clay Science, 2021, 212, 106221.	5.2	6
45	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
46	Interaction at the nanoscale of fundamental biological molecules with minerals. Advances in Nano Research, 2013, 1, 133-151.	0.9	5
47	Mineral surface-organic matter interactions: basics and applications. IOP Conference Series: Materials Science and Engineering, 2012, 32, 012027.	0.6	4
48	Elastic properties of heterodesmic composite structures: The case of calcite CaCO ₃ (space group) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 Part C: Open Access, 2021, 6, 100184.	3.2	4
49	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
50	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
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 from ab initio quantum 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	Fibre-Reinforced Geopolymer Composites Micro-Nanochemistry by SEM-EDS Simulations. Journal of Composites Science, 2021, 5, 214.	3.0	1
56	Preface to StSPM2019EV special issue. Journal of Microscopy, 2020, 280, 181-182.	1.8	0
57	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