

# Gianfranco Ulian

## List of Publications by Year in descending order

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63  
papers

795  
citations

471509

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docs citations

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times ranked

460  
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#	ARTICLE	IF	CITATIONS
1	Study of the variation of the optical properties of calcite with applied stress, useful for specific rock and material mechanics. <i>Scientific Reports</i> , 2022, 12, 299.	3.3	4
2	<i>QUANTAS</i> : a Python software for the analysis of thermodynamics and elastic behavior of solids from <i>ab initio</i> quantum mechanical simulations and experimental data. <i>Journal of Applied Crystallography</i> , 2022, 55, 386-396.	4.5	3
3	Structural and elastic behaviour of aragonite at high-pressure: A contribution from first-principle simulations. <i>Computational Materials Science</i> , 2022, 212, 111600.	3.0	3
4	Electronic and optical properties of graphene/molybdenite bilayer composite. <i>Composite Structures</i> , 2021, 255, 112978.	5.8	12
5	SEM-EDS nanoanalysis of mineral composite materials: A Monte Carlo approach. <i>Composite Structures</i> , 2021, 259, 113227.	5.8	4
6	Benchmarking dispersion-corrected DFT methods for the evaluation of materials with anisotropic properties: structural, electronic, dielectric, optical and vibrational analysis of calcite ( $\text{CaCO}_3$ , space group $R\bar{3}c$ ). <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18899-18907.	2.8	16
7	Development of A Nano-Apatite Based Composite Sealer for Endodontic Root Canal Filling. <i>Journal of Composites Science</i> , 2021, 5, 30.	3.0	3
8	Thermodynamic, elastic, and vibrational (IR/Raman) behavior of mixed type-AB carbonated hydroxylapatite by density functional theory. <i>American Mineralogist</i> , 2021, 106, 1928-1939.	1.9	7
9	Mineral diagnostics: SEM-EDS Monte Carlo strategy for optimised measurements of ultrathin fragments in Cultural Heritage studies. <i>Acta IMEKO (2012)</i> , 2021, 10, 193.	0.7	1
10	In Vivo Effects of Two In-Office Vital Tooth Bleaching Systems on Enamel Permeability. <i>Journal of Composites Science</i> , 2021, 5, 98.	3.0	1
11	DFT Simulation of the Water Molecule Interaction with the (001) Surface of Montmorillonite. <i>Minerals (Basel, Switzerland)</i> , 2021, 11, 501.	2.0	7
12	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
13	In Vitro Comparison of Root Surface Treatment Effect between Root Scaling with Ultrasonic Inserts and Gracey Curette and Polishing with Different Cleaning Pastes. <i>Applied Sciences (Switzerland)</i> , 2021, 11, 5967.	2.5	0
14	Fibre-Reinforced Geopolymer Composites Micro-Nanochemistry by SEM-EDS Simulations. <i>Journal of Composites Science</i> , 2021, 5, 214.	3.0	1
15	Monte Carlo strategy for SEM-EDS micro-nanoanalysis of geopolymer composites. <i>Composites Part C: Open Access</i> , 2021, 6, 100183.	3.2	1
16	Water adsorption behaviour on (001) pyrophyllite surface from <i>ab initio</i> Density Functional Theory simulations. <i>Applied Clay Science</i> , 2021, 212, 106221.	5.2	6
17	Elastic properties of heterodesmic composite structures: The case of calcite $\text{CaCO}_3$ (space group) $T\bar{1}Qq1$ 10.784314 $rgBT$ / <i>Overlook Part C: Open Access</i> , 2021, 6, 100184.	3.2	4
18	Thermal, X-ray Diffraction and Oedometric Analyses of Silt-Waste/NaOH-Activated Metakaolin Geopolymer Composite. <i>Journal of Composites Science</i> , 2021, 5, 269.	3.0	4

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19	First principle investigation of the thermomechanical properties of type A carbonated apatite. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26069.	2.0	8
20	Monte Carlo SEM-EDS Nano-Microanalysis Strategy of Historical Mineral Pigments: The Simulation of the Egyptian Blue from Pompeii (Italy) as an Example. <i>Minerals (Basel, Switzerland)</i> , 2020, 10, 807.	2.0	3
21	Nanoscale oligopeptide adsorption behaviour on chlorite as revealed by scanning probe microscopy and density functional simulations. <i>Applied Clay Science</i> , 2020, 197, 105777.	5.2	5
22	Thermodynamic and thermoelastic properties of wurtzite-ZnS by density functional theory. <i>American Mineralogist</i> , 2020, 105, 1212-1222.	1.9	7
23	Infrared and Raman spectroscopic features of clinochlore Mg <sub>6</sub> Si <sub>4</sub> O <sub>10</sub> (OH) <sub>8</sub> : A density functional theory contribution. <i>Applied Clay Science</i> , 2020, 197, 105779.	5.2	13
24	Simulated infrared and Raman spectroscopy, complex dielectric function and refractive index dataset of monoclinic C2/m stoichiometric clinochlore Mg <sub>6</sub> Si <sub>4</sub> O <sub>10</sub> (OH) <sub>8</sub> as obtained from Density Functional Theory. <i>Data in Brief</i> , 2020, 32, 106208.	1.0	1
25	Nano-atomic scale hydrophobic/philic confinement of peptides on mineral surfaces by cross-correlated SPM and quantum mechanical DFT analysis. <i>Journal of Microscopy</i> , 2020, 280, 204-221.	1.8	7
26	Thermodynamic and thermoelastic data of georesources raw minerals: Zinc sulphide and apatite. <i>Data in Brief</i> , 2020, 29, 105265.	1.0	3
27	Equation of state and second-order elastic constants of portlandite Ca(OH) <sub>2</sub> and brucite Mg(OH) <sub>2</sub> . <i>Physics and Chemistry of Minerals</i> , 2019, 46, 101-117.	0.8	16
28	3D meso-nanostructures in cleaved and nanolithographed Mg-Al-hydroxysilicate (clinochlore): Topology, crystal-chemistry, and surface properties. <i>Applied Clay Science</i> , 2019, 169, 74-80.	5.2	11
29	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
30	Thermomechanical, electronic and thermodynamic properties of ZnS cubic polymorphs: an ab initio 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
31	Equation of state of hexagonal hydroxylapatite (P <sub>6</sub> <sub>3</sub> ) as obtained from density functional theory simulations. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25553.	2.0	15
32	First principle investigation of the mechanical properties of natural layered nanocomposite: Clinochlore as a model system for heterodesmic structures. <i>Composite Structures</i> , 2018, 202, 551-558.	5.8	22
33	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. <i>Data in Brief</i> , 2018, 18, 325-333.	1.0	3
34	Second-order elastic constants of hexagonal hydroxylapatite (P <sub>6</sub> <sub>3</sub> ) from ab initio quantum mechanics: Comparison between DFT functionals and basis sets. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25500.	2.0	19
35	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
36	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

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37	Anisotropy and directional elastic behavior data obtained from the second-order elastic constants of portlandite Ca(OH) <sub>2</sub> and brucite Mg(OH) <sub>2</sub> . Data in Brief, 2018, 21, 1375-1380.	1.0	2
38	Crystal-chemical and structural data related to the equation of state and second-order elastic constants of portlandite Ca(OH) <sub>2</sub> and brucite Mg(OH) <sub>2</sub> . Data in Brief, 2018, 21, 2367-2375.	1.0	3
39	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
40	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
41	Nanomorphological investigation of graphite surface after cryo-ultrasonication in liquid nitrogen by atomic force microscopy. Micro and Nano Letters, 2018, 13, 546-551.	1.3	2
42	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
43	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
44	Effects of fluorine content on the elastic behavior of topaz [Al <sub>2</sub> SiO <sub>4</sub> (F,OH) <sub>2</sub> ]. American Mineralogist, 2017, 102, 347-356.	1.9	27
45	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
46	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
47	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
48	Density functional investigation of the thermophysical and thermochemical properties of talc [Mg <sub>3</sub> Si <sub>4</sub> O <sub>10</sub> (OH) <sub>2</sub> ]. Physics and Chemistry of Minerals, 2015, 42, 151-162.	0.8	31
49	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
50	Single Molecule Investigation of Glycine-Chlorite Interaction by Cross-Correlated Scanning Probe Microscopy and Quantum Mechanics Simulations. Langmuir, 2015, 31, 4453-4463.	3.5	21
51	Density functional investigation of the thermo-physical and thermo-chemical properties of 2M1 muscovite. American Mineralogist, 2015, 100, 935-944.	1.9	34
52	The compressional behaviour and the mechanical properties of talc [Mg <sub>3</sub> Si <sub>4</sub> O <sub>10</sub> (OH) <sub>2</sub> ]: a density functional theory investigation. Physics and Chemistry of Minerals, 2014, 41, 639-650.	0.8	34
53	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
54	Scanning probe atomic force microscopy: new developments and applications. IOP Conference Series: Materials Science and Engineering, 2014, 55, 012019.	0.6	0

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55	CO <sub>3</sub> <sup>2-</sup> Mobility in Carbonate Apatite As Revealed by Density Functional Modeling. Journal of Physical Chemistry C, 2014, 118, 1364-1369.	3.1	20
56	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
57	The vibrational features of hydroxylapatite and type A carbonated apatite: A first principle contribution. American Mineralogist, 2013, 98, 752-759.	1.9	55
58	Comparison between Gaussian-type orbitals and plane wave <i>ab initio</i> density functional theory modeling of layer silicates: Talc [Mg <sub>3</sub> Si <sub>4</sub> O <sub>10</sub> (OH) <sub>2</sub> ] as model system. Journal of Chemical Physics, 2013, 139, 204101.	3.0	44
59	Interaction at the nanoscale of fundamental biological molecules with minerals. Advances in Nano Research, 2013, 1, 133-151.	0.9	5
60	Scanning probe microscopy with vertically oriented cantilevers made easy. Measurement Science and Technology, 2012, 23, 085903.	2.6	5
61	Mineral surface-organic matter interactions: basics and applications. IOP Conference Series: Materials Science and Engineering, 2012, 32, 012027.	0.6	4
62	Nucleotides, RNA and DNA selective adsorption on atomic-flat Mg-Al-hydroxysilicate substrates. Micro and Nano Letters, 2011, 6, 922.	1.3	16
63	Interaction of organic molecules with layer silicates, oxides and hydroxides and related surface-nano-characterization techniques. , 2011, , 313-334.		4