Francisco Colmenero Ruiz

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8817148/publications.pdf

Version: 2024-02-01

44 papers	1,228 citations	361045 20 h-index	360668 35 g-index
44 all docs	44 docs citations	44 times ranked	456 citing authors

#	Article	IF	Citations
1	Approximatingq-order reduced density matrices in terms of the lower-order ones. II. Applications. Physical Review A, 1993, 47, 979-985.	1.0	192
2	Approximatingq-order reduced density matrices in terms of the lower-order ones. I. General relations. Physical Review A, 1993, 47, 971-978.	1.0	137
3	Self-consistent approximate solution of the second-order contracted SchrÃ¶dinger equation. International Journal of Quantum Chemistry, 1994, 51, 369-388.	1.0	110
4	Periodic Density Functional Theory Study of the Structure, Raman Spectrum, and Mechanical Properties of Schoepite Mineral. Inorganic Chemistry, 2018, 57, 4470-4481.	1.9	51
5	Study of the thermal stability of studtite by in situ Raman spectroscopy and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 174, 245-253.	2.0	46
6	Spectroscopic Raman characterization of rutherfordine: a combined DFT and experimental study. Physical Chemistry Chemical Physics, 2016, 18, 16575-16584.	1.3	43
7	Density Functional Theory Study of the Thermodynamic and Raman Vibrational Properties of Î³-UO₃ Polymorph. Journal of Physical Chemistry C, 2017, 121, 14507-14516.	1.5	43
8	Mechanical properties of anhydrous oxalic acid and oxalic acid dihydrate. Physical Chemistry Chemical Physics, 2019, 21, 2673-2690.	1.3	43
9	Thermodynamic and Mechanical Properties of the Rutherfordine Mineral Based on Density Functional Theory. Journal of Physical Chemistry C, 2017, 121, 5994-6001.	1.5	41
10	Structural, mechanical and vibrational study of uranyl silicate mineral soddyite by DFT calculations. Journal of Solid State Chemistry, 2017, 253, 249-257.	1.4	39
11	Becquerelite mineral phase: crystal structure and thermodynamic and mechanical stability by using periodic DFT. RSC Advances, 2018, 8, 24599-24616.	1.7	36
12	Temperature-Dependent Gibbs Free Energies of Reaction of Uranyl-Containing Materials Based on Density Functional Theory. Journal of Physical Chemistry C, 2018, 122, 5268-5279.	1.5	34
13	Thermodynamic Properties of Uranyl-Containing Materials Based on Density Functional Theory. Journal of Physical Chemistry C, 2018, 122, 5254-5267.	1.5	32
14	Periodic DFT Study of the Thermodynamic Properties and Stability of Schoepite and Metaschoepite Mineral Phases. ACS Earth and Space Chemistry, 2019, 3, 17-28.	1.2	26
15	Organic acids under pressure: elastic properties, negative mechanical phenomena and pressure induced phase transitions in the lactic, maleic, succinic and citric acids. Materials Advances, 2020, 1, 1399-1426.	2.6	25
16	Crystal structure, hydrogen bonding, mechanical properties and Raman spectrum of the lead uranyl silicate monohydrate mineral kasolite. RSC Advances, 2019, 9, 15323-15334.	1.7	24
17	Study of the structural, vibrational and thermodynamic properties of natroxalate mineral using density functional theory. Journal of Solid State Chemistry, 2018, 263, 131-140.	1.4	23
18	Silver Oxalate: Mechanical Properties and Extreme Negative Mechanical Phenomena. Advanced Theory and Simulations, 2019, 2, 1900040.	1.3	23

#	Article	IF	Citations
19	Anomalous mechanical behavior of the deltic, squaric and croconic cyclic oxocarbon acids. Materials Research Express, 2019, 6, 045610.	0.8	23
20	Structural, mechanical and Raman spectroscopic characterization of the layered uranyl silicate mineral, uranophane-Î±, by density functional theory methods. Clay Minerals, 2018, 53, 377-392.	0.2	20
21	The layered uranyl silicate mineral uranophane-Î²: crystal structure, mechanical properties, Raman spectrum and comparison with the Î±-polymorph. Dalton Transactions, 2019, 48, 16722-16736.	1.6	20
22	Negative area compressibility in oxalic acid dihydrate. Materials Letters, 2019, 245, 25-28.	1.3	17
23	Extreme negative mechanical phenomena in the zinc and cadmium anhydrous metal oxalates and lead oxalate dihydrate. Journal of Materials Science, 2020, 55, 218-236.	1.7	17
24	Revealing Rutherfordine Mineral as an Auxetic Material. Applied Sciences (Switzerland), 2018, 8, 2281.	1.3	15
25	Structural, spectroscopic, and thermodynamic characterization of ammonium oxalate monohydrate mineral using theoretical solid-state methods. Journal of Physics and Chemistry of Solids, 2019, 125, 31-42.	1.9	14
26	Thermodynamic, Raman Spectroscopic, and UVâ€“Visible Optical Characterization of the Deltic, Squaric, and Croconic Cyclic Oxocarbon Acids. Journal of Physical Chemistry A, 2019, 123, 4241-4261.	1.1	13
27	Periodic density functional theory study of the Raman spectrum of the hydrated uranyl oxyhydroxide mineral becquerelite. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	12
28	Negative linear compressibility in uranyl squarate monohydrate. Journal of Physics Condensed Matter, 2019, 31, 175701.	0.7	11
29	Thermodynamic properties of the uranyl carbonate minerals roubaultite, fontanite, widenmannite, grimselite, Äejkaite and bayleyite. Inorganic Chemistry Frontiers, 2020, 7, 4160-4179.	3.0	11
30	Uranosphaerite: Crystal structure, hydrogen bonding, mechanics, infrared and Raman spectroscopy and thermodynamics. Journal of Physics and Chemistry of Solids, 2020, 141, 109400.	1.9	11
31	Negative area compressibility in silver oxalate. Journal of Materials Science, 2021, 56, 269-277.	1.7	11
32	Structural, mechanical, spectroscopic and thermodynamic characterization of the copper-uranyl tetrahydroxide mineral vandenbrandeite. RSC Advances, 2019, 9, 40708-40726.	1.7	10
33	Crystal Structure, Infrared Spectrum and Elastic Anomalies in Tuperssuatsiaite. Scientific Reports, 2020, 10, 7510.	1.6	10
34	Full crystal structure, hydrogen bonding and spectroscopic, mechanical and thermodynamic properties of mineral uranopilite. RSC Advances, 2020, 10, 31947-31960.	1.7	10
35	Negative linear compressibility in nanoporous metalâ€“organic frameworks rationalized by the empty channel structural mechanism. Physical Chemistry Chemical Physics, 2021, 23, 8508-8524.	1.3	9
36	The crystal structures and mechanical properties of the uranyl carbonate minerals roubaultite, fontanite, sharpite, widenmannite, grimselite and Äejkaite. Inorganic Chemistry Frontiers, 2020, 7, 4197-4221.	3.0	9

#	Article	IF	Citations
37	Addendum: anomalous mechanical behavior of the deltic, squaric and croconic cyclic oxocarbon acids. Materials Research Express, 2019, 6, 069401.	0.8	7
38	The magnesium uranyl tricarbonate octadecahydrate mineral, bayleyite: Periodic DFT study of its crystal structure, hydrogen bonding, mechanical properties and infrared spectrum. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 234, 118216.	2.0	6
39	Compressing the Channels in the Crystal Structure of Copper Squarate Metal-Organic Framework. Solids, 2022, 3, 374-384.	1.1	2
40	Mechanical anomalies in mercury oxalate and the deformation of the mercury cube coordination environment under pressure. Applied Physics A: Materials Science and Processing, 2021, 127, 1.	1.1	1
41	Fluorine-substituted cyclobutenes in the solid state: Crystal structures, vibrational spectra and mechanical and thermodynamic properties. Journal of Physics and Chemistry of Solids, 2022, 160, 110337.	1.9	1
42	Graphical method for operating in second quantization. Physical Review A, 1994, 49, 4217-4220.	1.0	0
43	The Application of Periodic Density Functional Theory to the Study of Uranyl-Containing Materials: Thermodynamic Properties and Stability. , 2019, , .		0
44	Theoretical Studies of the Structural, Mechanical and Raman Spectroscopic Properties of Uranyl-Containing Minerals. , 0, , .		0