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List of Publications by Year
in descending order

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Version: 2024-02-01

54 papers	964 citations	430874 18 h-index	477307 29 g-index
54 all docs	54 docs citations	54 times ranked	1057 citing authors

#	Article	IF	Citations
1	An Atomistic Model Describing the Structure and Morphology of Cu-Doped C-S-H Hardening Accelerator Nanoparticles. Nanomaterials, 2022, 12, 342.	4.1	9
2	Calcite/Aragonite Epitaxy: A Computational Study for Understanding Mollusk Shell Formation. Journal of Physical Chemistry C, 2022, 126, 6472-6481.	3.1	3
3	Epitaxy: a methodological approach to the study of an old phenomenon. CrystEngComm, 2022, 24, 4165-4173.	2.6	5
4	Epitaxies of Ca-sulfates on calcite (CaCO₃) I. Gypsum {010} on the calcite {10.4} form: epi-twins of gypsum induced by the calcite substrate. CrystEngComm, 2022, 24, 5120-5127.	2.6	4
5	A new computational strategy to calculate the surface energy of a dipolar crystal surface. CrystEngComm, 2021, 23, 4791-4798.	2.6	2
6	Growth and Equilibrium Morphology of Hydrohalite (NaClÂ·2H2O) and Its Epitaxy with Hexagonal Ice Crystals. Journal of Physical Chemistry C, 2021, 125, 6923-6932.	3.1	1
7	Theoretical equilibrium shape of hydroxyapatite, revised. CrystEngComm, 2020, 22, 7944-7951.	2.6	1
8	The influence of Caâ€“Mg disorder on the growth of dolomite: a computational study. CrystEngComm, 2020, 22, 4853-4861.	2.6	8
9	Impurity Effects on Habit Change and Polymorphic Transitions in the System: Aragoniteâ€“Calciteâ€“Vaterite. Crystal Growth and Design, 2020, 20, 2497-2507.	3.0	11
10	Equilibrium Shape of 2D Nuclei Obtained from Spiral Hillocks on {010} Form of Gypsum. Crystal Growth and Design, 2020, 20, 1526-1530.	3.0	3
11	A two-step nucleation model based on diffuse interface theory (DIT) to explain the non-classical view of calcium carbonate polymorph formation. CrystEngComm, 2019, 21, 4918-4924.	2.6	10
12	Adsorption/Absorption of Lithium Affecting the Growth Morphology of Aragonite. The Two-Dimensional Epitaxy of Li₂CO₃ (Zabuyelite) on the {001} Form of Aragonite (CaCO₃). Crystal Growth and Design, 2019, 19, 3969-3978.	3.0	4
13	Structure and adhesion energy of the (10.4) calcite/(001) ice Ih and (210) baryte/(001) ice Ih interfaces. CrystEngComm, 2019, 21, 2920-2928.	2.6	3
14	Ab Initio Calculations of the Main Crystal Surfaces of Baryte (BaSO₄). Crystal Growth and Design, 2018, 18, 4084-4094.	3.0	10
15	BaCO₃ and NH₃SO₃ as precursors for the hydrothermal synthesis of BaSO₄. CrystEngComm, 2018, 20, 7001-7009.	2.6	1
16	Habit Change of Monoclinic Hydroxyapatite Crystals Growing from Aqueous Solution in the Presence of Citrate Ions: The Role of 2D Epitaxy. Crystals, 2018, 8, 308.	2.2	16
17	(10.4) Face of Ordered and Disordered Dolomite, MgCa(CO3)2: A Computational Study to Reveal the Growth Mechanism. Minerals (Basel, Switzerland), 2018, 8, 323.	2.0	7
18	The effect of impurities on the structure and energy of a crystal surface: Mg impurities in calcite as a case study. CrystEngComm, 2018, 20, 4556-4564.	2.6	5

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19	A revised thermodynamic model for crystal surfaces. I. Theoretical aspects. CrystEngComm, 2017, 19, 6314-6324.	2.6	3
20	A new computational approach to the study of epitaxy: the calcite/dolomite case. CrystEngComm, 2017, 19, 3939-3946.	2.6	8
21	About the Genetic Mechanisms of Apatites: A Survey on the Methodological Approaches. Minerals (Basel, Switzerland), 2017, 7, 139.	2.0	16
22	Behavior of the Chemical Potential in Calcite and Magnesite Crystals: A Damped Harmonic Oscillation. Crystal Growth and Design, 2016, 16, 2671-2677.	3.0	11
23	Elastic properties of the (001) face of xenon crystals. Colloid Journal, 2016, 78, 658-668.	1.3	1
24	X-ray topographic study of a diamond from Udachnaya: Implications for the genetic nature of inclusions. Lithos, 2016, 248-251, 153-159.	1.4	23
25	Diamond and its olivine inclusions: A strange relation revealed by ab initio simulations. Earth and Planetary Science Letters, 2016, 435, 31-35.	4.4	20
26	Firstâ€principle modelling of forsterite surface properties: Accuracy of methods and basis sets. Journal of Computational Chemistry, 2015, 36, 1439-1445.	3.3	14
27	Twin Laws and Energy in Monoclinic Hydroxyapatite, Ca₅(PO₄)₃(OH). Crystal Growth and Design, 2015, 15, 411-418.	3.0	13
28	Computational Approach to the Study of Epitaxy: Natural Occurrence in Diamond/Forsterite and Aragonite/Zabuyelite. Crystal Growth and Design, 2015, 15, 2979-2987.	3.0	12
29	The free energy density of a crystal: calcite (CaCO3) as a case of study. CrystEngComm, 2015, 17, 2204-2211.	2.6	23
30	Olivine with diamond-imposed morphology included in diamonds. Syngenesis or protogenesis?. International Geology Review, 2014, 56, 1658-1667.	2.1	59
31	Low Symmetry Polymorph of Hydroxyapatite. Theoretical Equilibrium Morphology of the Monoclinic Ca₅(OH)(PO₄)₃. Crystal Growth and Design, 2014, 14, 2846-2852.	3.0	26
32	Analysis of the Configurations of a Crystal Surface. Pyrope (Mg₃Al₂Si₃O₁₂) as a Case Study. Crystal Growth and Design, 2014, 14, 2357-2365.	3.0	7
33	Surface structure, morphology and (110) twin of aragonite. CrystEngComm, 2014, 16, 627-635.	2.6	11
34	Configurational and energy study of the (100) and (110) surfaces of the MgAl₂O₄spinel by means of quantum mechanical and empirical techniques. CrystEngComm, 2014, 16, 9224-9235.	2.6	10
35	Ab Initio Calculations of the Main Crystal Surfaces of Forsterite (Mg₂SiO₄): A Preliminary Study to Understand the Nature of Geochemical Processes at the Olivine Interface. Journal of Physical Chemistry C, 2014, 118, 2498-2506.	3.1	48
36	The (100), (111) and (110) surfaces of diamond: anab initioB3LYP study. Molecular Physics, 2014, 112, 1030-1039.	1.7	55

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37	A new calculation strategy to analyze the vibrational free energy of a slab and calculate the vibrational contribution of the surface free energy. CrystEngComm, 2013, 15, 6736.	2.6	16
38	New Estimates of the Free Energy of Calcite/Water Interfaces for Evaluating the Equilibrium Shape and Nucleation Mechanisms. Crystal Growth and Design, 2013, 13, 1170-1179.	3.0	49
39	The reconstruction of dipolar surfaces: a preliminary step for adsorption modeling. Crystal Research and Technology, 2013, 48, 811-818.	1.3	13
40	Theoretical Equilibrium Shape of Calcite. 2. [4ì...41] Zone and Its Role in Biomineralization. Crystal Growth and Design, 2011, 11, 3985-3993.	3.0	27
41	Pyroxene inclusions in paleo-Christian mosaic tesserae: a new tool for constraining the glass manufacturing temperature. Applied Physics A: Materials Science and Processing, 2011, 103, 207-212.	2.3	4
42	(10.4), (01.8), (01.2), and (00.1) Twin Laws of Calcite (CaCO₃): Equilibrium Geometry of the Twin Boundary Interfaces and Twinning Energy. Crystal Growth and Design, 2010, 10, 3102-3109.	3.0	41
43	Effect of the Surface Relaxation on the Theoretical Equilibrium Shape of Calcite. 1. The [001] Zone. Crystal Growth and Design, 2010, 10, 4096-4100.	3.0	18
44	Surface reconstructions and relaxation effects in a centre-symmetrical crystal: the {00.1} form of calcite (CaCO3). CrystEngComm, 2010, 12, 3626.	2.6	38
45	{100} and {111} forms of the NaCl crystals coexisting in growth from pure aqueous solution. Journal of Crystal Growth, 2009, 311, 399-403.	1.5	37
46	Quantum-Mechanical and Thermodynamical Study on the (110) and Reconstructed (111) Faces of NaCl Crystals. Crystal Growth and Design, 2009, 9, 1912-1916.	3.0	23
47	Quantum-Mechanical and Thermodynamical Study on the (100) Face of LiF Crystals. Crystal Growth and Design, 2009, 9, 404-408.	3.0	8
48	Thermal expansion along the NaAlSi2O6â€“NaFe3+Si2O6 and NaAlSi2O6â€“CaFe2+Si2O6 solid solutions. Physics and Chemistry of Minerals, 2008, 35, 241-248.	0.8	22
49	Theoretical structure and surface energy of the reconstructed {01.2} form of calcite (CaCO3) crystal. Surface Science, 2008, 602, 2774-2782.	1.9	35
50	Structures and Surface Energies of (100) and Octopolar (111) Faces of Halite (NaCl): an Ab initio Quantum-Mechanical and Thermodynamical Study. Crystal Growth and Design, 2008, 8, 2163-2170.	3.0	46
51	Ab initio quantum-mechanical modeling of the (001), and (110) surfaces of zabuyelite (Li2CO3). Surface Science, 2007, 601, 3012-3019.	1.9	34
52	Neutral sodium atoms release from the surfaces of the Moon and Mercury induced by meteoroid impacts. Planetary and Space Science, 2007, 55, 1494-1501.	1.7	27
53	Morphology of Calcite (CaCO3) Crystals Growing from Aqueous Solutions in the Presence of Li+Ions. Surface Behavior of the {0001} Form. Crystal Growth and Design, 2004, 4, 485-490.	3.0	63
54	A new computational strategy to calculate the edge energy of a relaxed step. Calcite (CaCO3) as a case study. CrystEngComm, 0, , .	2.6	0