Alexey A Sokol

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7265918/publications.pdf

Version: 2024-02-01

119 papers	7,308 citations	76196 40 h-index	54797 84 g-index
142 all docs	142 docs citations	142 times ranked	10112 citing authors

#	Article	IF	Citations
1	Materials and Molecular Modeling at the Exascale. Computing in Science and Engineering, 2022, 24, 36-45.	1.2	7
2	Insight into the Fergusoniteâ€“Scheelite Phase Transition of ABO₄-Type Oxides by Density Functional Theory: A Case Study of the Subtleties of the Ground State of BiVO₄. Chemistry of Materials, 2022, 34, 5334-5343.	3.2	6
3	A computational investigation of the adsorption of small copper clusters on the CeO₂(110) surface. Physical Chemistry Chemical Physics, 2021, 23, 19329-19342.	1.3	7
4	The Interplay of Interstitial and Substitutional Copper in Zinc Oxide. Frontiers in Chemistry, 2021, 9, 780935.	1.8	4
5	Morphology of Cu clusters supported on reconstructed polar ZnO (0001) and (0001Ì„) surfaces. Journal of Materials Chemistry A, 2020, 8, 22840-22857.	5.2	9
6	Real and virtual polymorphism of titanium selenide with robust interatomic potentials. Journal of Materials Chemistry A, 2020, 8, 14054-14061.	5.2	8
7	Are octahedral clusters missing on the carbon energy landscape?. Nanoscale Advances, 2019, 1, 89-93.	2.2	6
8	Donor and acceptor characteristics of native point defects in GaN. Journal Physics D: Applied Physics, 2019, 52, 335104.	1.3	49
9	Hybrid-DFT Modeling of Lattice and Surface Vacancies in MnO. Journal of Physical Chemistry C, 2019, 123, 8133-8144.	1.5	10
10	Open-Source, Python-Based Redevelopment of the ChemShell Multiscale QM/MM Environment. Journal of Chemical Theory and Computation, 2019, 15, 1317-1328.	2.3	46
11	Thermodynamically accessible titanium clusters Ti_N, N = 2â€“32. Physical Chemistry Chemical Physics, 2018, 20, 13962-13973.	1.3	18
12	Defect formation in In₂O₃and SnO₂: a new atomistic approach based on accurate lattice energies. Journal of Materials Chemistry C, 2018, 6, 12386-12395.	2.7	42
13	Oxidation states and ionicity. Nature Materials, 2018, 17, 958-964.	13.3	135
14	Prediction of multiband luminescence due to the gallium vacancyâ€“oxygen defect complex in GaN. Applied Physics Letters, 2018, 112, .	1.5	25
15	What is the best or most relevant global minimum for nanoclusters? Predicting, comparing and recycling cluster structures with WASP@N. Faraday Discussions, 2018, 211, 593-611.	1.6	6
16	Deep vs shallow nature of oxygen vacancies and consequent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>n</mml:mi></mml:math>-type carrier concentrations in transparent conducting oxides. Physical Review Materials, 2018, 2, .	0.9	73
17	An efficient genetic algorithm for structure prediction at the nanoscale. Nanoscale, 2017, 9, 3850-3864.	2.8	35
18	Heterostructures of GaN with SiC and ZnO enhance carrier stability and separation in framework semiconductors. Physica Status Solidi (A) Applications and Materials Science, 2017, 214, 1600440.	0.8	7

#	Article	IF	Citations
19	Why Are Polar Surfaces of ZnO Stable?. Chemistry of Materials, 2017, 29, 5306-5320.	3.2	141
20	Electron Counting in Solids: Oxidation States, Partial Charges, and Ionicity. Journal of Physical Chemistry Letters, 2017, 8, 2074-2075.	2.1	65
21	Demonstration of the donor characteristics of Si and O defects in GaN using hybrid QM/MM. Physica Status Solidi (A) Applications and Materials Science, 2017, 214, 1600445.	0.8	16
22	Magnetic coupling constants for MnO as calculated using hybrid density functional theory. Chemical Physics Letters, 2017, 690, 47-53.	1.2	5
23	Ising-like antiferromagnetism on the octahedral sublattice of a cobalt-containing garnet and the potential for quantum criticality. Physical Review B, 2017, 95, .	1.1	8
24	Development of Interatomic Potentials for Supported Nanoparticles: The Cu/ZnO Case. Journal of Physical Chemistry C, 2017, 121, 16831-16844.	1.5	19
25	Nonstoichiometry and Weyl fermionic behavior in TaAs. Physical Review B, 2016, 94, .	1.1	20
26	Modelling the chemistry of Mn-doped MgO for bulk and (100) surfaces. Physical Chemistry Chemical Physics, 2016, 18, 28648-28660.	1.3	11
27	Anharmonicity in the High-Temperature<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>C</mml:mi><mml:mi>m</mml:mi><mml:mi>c</mml:mi><mml:mi>m</mml:mi></mml:math>Phase of SnSe: Soft Modes and Three-Phonon Interactions. Physical Review Letters, 2016, 117, 075502.	2.9	147
28	Modelling metal centres, acid sites and reaction mechanisms in microporous catalysts. Faraday Discussions, 2016, 188, 235-255.	1.6	29
29	Bulk electronic, elastic, structural, and dielectric properties of the Weyl semimetal TaAs. Physical Review B, 2016, 93, .	1.1	42
30	Double bubble secondary building units used as a structural motif for enhanced electronâ€“hole separation in solids. Materials Science in Semiconductor Processing, 2016, 42, 147-149.	1.9	4
31	One-Dimensional Nanosystems. Series in Materials Science and Engineering, 2016, , 47-81.	0.1	1
32	Antiferromagnetism atT>500Kin the layered hexagonal ruthenateSrRu2O6. Physical Review B, 2015, 92, .	1.1	43
33	BuckeridgeetÂal.Reply:. Physical Review Letters, 2015, 115, 029702.	2.9	6
34	Morphological Features and Band Bending at Nonpolar Surfaces of ZnO. Journal of Physical Chemistry C, 2015, 119, 11598-11611.	1.5	33
35	Determination of the Nitrogen Vacancy as a Shallow Compensating Center in GaN Doped with Divalent Metals. Physical Review Letters, 2015, 114, 016405.	2.9	70
36	Polymorph Engineering of TiO₂: Demonstrating How Absolute Reference Potentials Are Determined by Local Coordination. Chemistry of Materials, 2015, 27, 3844-3851.	3.2	113

#	Article	IF	Citations
37	Structural, energetic and electronic properties of (100) surfaces for alkaline earth metal oxides as calculated with hybrid density functional theory. Surface Science, 2015, 642, 58-65.	0.8	18
38	From Stable ZnO and GaN Clusters to Novel Double Bubbles and Frameworks. Inorganics, 2014, 2, 248-263.	1.2	10
39	Embedded-cluster calculations in a numeric atomic orbital density-functional theory framework. Journal of Chemical Physics, 2014, 141, 024105.	1.2	38
40	<scp>C</scp>hem<scp>S</scp>hellâ€"a modular software package for <scp>QM</scp>/<scp>MM</scp> simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 101-110.	6.2	351
41	From monomer to monolayer: a global optimisation study of (ZnO)_n nanoclusters on the Ag surface. Nanoscale, 2014, 6, 14754-14765.	2.8	9
42	Double bubbles: a new structural motif for enhanced electronâ€"hole separation in solids. Physical Chemistry Chemical Physics, 2014, 16, 21098-21105.	1.3	11
43	The reactivity of CO₂and H₂at trapped electron sites at an oxide surface. Physical Chemistry Chemical Physics, 2014, 16, 21153-21156.	1.3	8
44	The reactivity of CO₂on the MgO(100) surface. Physical Chemistry Chemical Physics, 2014, 16, 184-195.	1.3	36
45	Bulk ionization potentials and band alignments from three-dimensional periodic calculations as demonstrated on rocksalt oxides. Physical Review B, 2014, 90, .	1.1	33
46	Interlayer Cation Exchange Stabilizes Polar Perovskite Surfaces. Advanced Materials, 2014, 26, 7252-7256.	11.1	36
47	Limits to Doping of Wide Band Gap Semiconductors. Chemistry of Materials, 2013, 25, 2924-2926.	3.2	57
48	Band alignment of rutile and anatase TiO2. Nature Materials, 2013, 12, 798-801.	13.3	1,924
49	Dynamical response and instability in ceria under lattice expansion. Physical Review B, 2013, 87, .	1.1	48
50	Structural and Optical Properties of Mg and Cd Doped ZnO Nanoclusters. Journal of Physical Chemistry C, 2013, 117, 27127-27145.	1.5	34
51	One-dimensional embedded cluster approach to modeling CdS nanowires. Journal of Chemical Physics, 2013, 139, 124101.	1.2	6
52	Magnetic properties of Fe2GeMo3N; an experimental and computational study. Journal of Materials Chemistry, 2012, 22, 15606.	6.7	5
53	Prediction on the existence and chemical stability of cuprous fluoride. Chemical Science, 2012, 3, 2565.	3.7	22
54	From Ergodicity to Extended Phase Diagrams. Angewandte Chemie - International Edition, 2012, 51, 3752-3754.	7.2	10

#	Article	IF	Citations
55	Activation of Carbon Dioxide over Zinc Oxide by Localised Electrons. ChemPhysChem, 2012, 13, 3453-3456.	1.0	34
56	Electron and hole stability in GaN and ZnO. Journal of Physics Condensed Matter, 2011, 23, 334217.	0.7	11
57	Microscopic origins of electron and hole stability in ZnO. Chemical Communications, 2011, 47, 3386.	2.2	54
58	Characterization of hydrogen dissociation over aluminium-doped zinc oxide using an efficient massively parallel framework for QM/MM calculations. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2011, 467, 1900-1924.	1.0	21
59	Potential energy landscapes for anion Frenkel-pair formation in ceria and india. Solid State Ionics, 2011, 184, 52-56.	1.3	29
60	Strontium migration assisted by oxygen vacancies in SrTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>from classical and quantum mechanical simulations. Physical Review B, 2011, 83, .	1.1	67
61	Free energy of defect formation: Thermodynamics of anion Frenkel pairs in indium oxide. Physical Review B, 2011, 83, .	1.1	24
62	Oxygen interstitial structures in close-packed metal oxides. Chemical Physics Letters, 2010, 492, 44-48.	1.2	48
63	Modelling nano-clusters and nucleation. Physical Chemistry Chemical Physics, 2010, 12, 786-811.	1.3	174
64	On the problem of cluster structure diversity and the value of data mining. Physical Chemistry Chemical Physics, 2010, 12, 8438.	1.3	30
65	Advances in computational studies of energy materials. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2010, 368, 3379-3456.	1.6	119
66	The effect of local environment on photoluminescence: A time-dependent density functional theory study of silanone groups on the surface of silica nanostructures. Journal of Chemical Physics, 2009, 131, 034705.	1.2	32
67	Physical Properties, Intrinsic Defects, and Phase Stability of Indium Sesquioxide. Chemistry of Materials, 2009, 21, 4962-4969.	3.2	61
68	Construction of nano- and microporous frameworks from octahedral bubble clusters. Physical Chemistry Chemical Physics, 2009, 11, 3176.	1.3	34
69	Bubbles and microporous frameworks of silicon carbide. Physical Chemistry Chemical Physics, 2009, 11, 3186.	1.3	44
70	Zinc oxide: A case study in contemporary computational solid state chemistry. Journal of Computational Chemistry, 2008, 29, 2234-2249.	1.5	105
71	Structures of Zinc Oxide Nanoclusters: As Found by Revolutionary Algorithm Techniques. Journal of Physical Chemistry C, 2008, 112, 18860-18875.	1.5	106
72	Hybrid QM/MM Investigations into the Structure and Properties of Oxygen-Donating Species in TS-1. Journal of Physical Chemistry C, 2008, 112, 7173-7185.	1.5	32

#	Article	IF	Citations
73	Structure, optical properties and defects in nitride (IIIâ€"V) nanoscale cage clusters. Physical Chemistry Chemical Physics, 2008, 10, 1944.	1.3	42
74	The Growth of Copper Clusters over ZnO:â€‰ the Competition between Planar and Polyhedral Clusters. Journal of Physical Chemistry C, 2008, 112, 7420-7430.	1.5	24
75	Defect structures in the silver halides. Physical Review B, 2008, 77, .	1.1	15
76	Optical excitations of defects in realistic nanoscale silica clusters: Comparing the performance of density functional theory using hybrid functionals with correlated wavefunction methods. Journal of Chemical Physics, 2008, 129, 014706.	1.2	11
77	Zinc oxide: A case study in contemporary computational solid state chemistry. , 2008, 29, 2234.		1
78	Point defects in ZnO. Faraday Discussions, 2007, 134, 267-282.	1.6	151
79	Formation of Active Sites in TS-1 by Hydrolysis and Inversion. Journal of Physical Chemistry C, 2007, 111, 14720-14731.	1.5	22
80	Computer Modelling in Solid-State Chemistry. , 2007, , 180-207.		1
81	Adsorption of Organosilanes at a Zn-Terminated ZnO (0001) Surface:Â Molecular Dynamics Study. Langmuir, 2006, 22, 8036-8042.	1.6	30
82	QM/MM modelling of the TS-1 catalyst using HPCx. Journal of Materials Chemistry, 2006, 16, 1919.	6.7	45
83	A Computational Investigation of the Different Intermediates during Organoalkoxysilane Hydrolysis. Journal of Physical Chemistry B, 2006, 110, 24311-24317.	1.2	3
84	Formation of Heteroatom Active Sites in Zeolites by Hydrolysis and Inversion. Angewandte Chemie - International Edition, 2006, 45, 1633-1638.	7.2	25
85	Electronic structure and magnetic coupling inFeSbO4: A DFT study using hybrid functionals andGGA+Umethods. Physical Review B, 2006, 73, .	1.1	43
86	Computational Approaches to the Determination of Active Site Structures and Reaction Mechanisms in Heterogeneous Catalysts. ChemInform, 2005, 36, no.	0.1	0
87	Hole localization in [AlO4]0 defects in silica materials. Journal of Chemical Physics, 2005, 122, 144704.	1.2	74
88	25ÂÂComputer modelling of inorganic materials. Annual Reports on the Progress of Chemistry Section A, 2005, , .	0.8	3
89	The nature of the oxidation states of gold on ZnO. Physical Chemistry Chemical Physics, 2005, 7, 2440.	1.3	35
90	Computational approaches to the determination of active site structures and reaction mechanisms in heterogeneous catalysts. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2005, 363, 913-936.	1.6	94

#	Article	IF	Citations
91	Transformation of hydroxyl nests in microporous aluminosilicates upon annealing. Journal of Physics Condensed Matter, 2004, 16, S2781-S2794.	0.7	15
92	Defect structures in silver chloride. Journal of Physics Condensed Matter, 2004, 16, S2827-S2838.	0.7	5
93	The RÃ1e of Defects in Photographic Latent Image Formation. Materials Research Society Symposia Proceedings, 2004, 848, 371.	0.1	2
94	Structure Prediction of Inorganic Nanoparticles with Predefined Architecture using a Genetic Algorithm. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2004, 630, 2343-2353.	0.6	51
95	Hybrid QM/MM embedding approach for the treatment of localized surface states in ionic materials. International Journal of Quantum Chemistry, 2004, 99, 695-712.	1.0	97
96	Interaction of adsorbed organosilanes with polar zinc oxide surfaces: a molecular dynamics study comparing two models for the metal oxide surface. Chemical Physics Letters, 2004, 393, 107-111.	1.2	41
97	Active sites for heterogeneous catalysis by functionalisation of internal and external surfaces. Catalysis Today, 2004, 93-95, 535-540.	2.2	11
98	The initial stages of aminosilanol polymerisation. Chemical Communications, 2004, , 20.	2.2	4
99	Identification and Characterization of Active Sites and Their Catalytic Processesâ€"the Cu/ZnO Methanol Catalyst. Topics in Catalysis, 2003, 24, 161-172.	1.3	87
100	Applications of Density Functional Theory in Solid State Chemistry. ChemInform, 2003, 34, no.	0.1	1
101	QUASI: A general purpose implementation of the QM/MM approach and its application to problems in catalysis. Computational and Theoretical Chemistry, 2003, 632, 1-28.	1.5	887
102	Assignment of the complex vibrational spectra of the hydrogenated ZnO polar surfaces using QM/MM embedding. Journal of Chemical Physics, 2003, 118, 317-320.	1.2	36
103	Understanding the interface between oxides and metals. Faraday Discussions, 2003, 124, 185.	1.6	28
104	Metal Cluster Support Interactions in the Cu/ZnO System:Â A QM/MM Study. Journal of Physical Chemistry B, 2003, 107, 7045-7057.	1.2	42
105	Local States in Microporous Silica and Aluminum Silicate Materials. 1. Modeling Structure, Formation, and Transformation of Common Hydrogen Containing Defects. Journal of Physical Chemistry B, 2002, 106, 6163-6177.	1.2	53
106	Surface structure of zinc oxide (), using an atomistic, semi-infinite treatment. Surface Science, 2002, 498, 135-146.	0.8	64
107	True Structure of Trigonal Bipyramidal SiO4F-Species in Siliceous Zeolites. Chemistry of Materials, 2001, 13, 4708-4713.	3.2	52
108	From CO2 to Methanol by Hybrid QM/MM Embedding This work was supported by EU Esprit IV project 25047. S.A.F. is grateful to ICI and Synetix for funding. K. Waugh, L. Whitmore, S. Cristol, and P. Sushko are thanked for their helpful insights. QM/MM=quantum mechanics/molecular mechanics.. Angewandte Chemie - International Edition, 2001, 40, 4437.	7.2	102

#	Article	IF	Citations
109	Novel Solid State Hybrid QM/MM Embedding Investigation into Methanol Synthesis over Cu Supported on ZnO Catalysts. Materials Research Society Symposia Proceedings, 2001, 677, 931.	0.1	0
110	From CO2 to Methanol by Hybrid QM/MM Embedding. , 2001, 40, 4437.		1
111	Computational Investigation into the Origins of Lewis Acidity in Zeolites. Advanced Materials, 2000, 12, 1801-1805.	11.1	25
112	Electron spin localisation and correlation effects for point defects in semi-ionic solids. Computational Materials Science, 2000, 17, 312-318.	1.4	7
113	Computer Modelling of Catalysts and Catalysis. , 2000, , 3-60.		1
114	A model for the formation of point defects in zeolites. Radiation Effects and Defects in Solids, 1999, 151, 235-241.	0.4	6
115	Defect Centers in Microporous Aluminum Silicate Materials. Journal of Physical Chemistry B, 1998, 102, 10647-10649.	1.2	20
116	Semi-empirical supercell calculations for free- and bound-hole polarons in crystal. Journal of Physics Condensed Matter, 1997, 9, 3559-3573.	0.7	4
117	Modelling Structure and Defects in Zeolites. , 1997, , 125-135.		2
118	Understanding the interface between oxides and metals. , 0, .		1
119	Assignment of the complex vibrational spectra of the hydrogenated ZnO polar surfaces using QM/MM embedding. , 0, .		1