Alexey A Sokol

List of Publications by Year
in descending order

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	Band alignment of rutile and anatase TiO2. Nature Materials, 2013, 12, 798-801.	13.3	1,924
2	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
3	<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
4	Modelling nano-clusters and nucleation. Physical Chemistry Chemical Physics, 2010, 12, 786-811.	1.3	174
5	Point defects in ZnO. Faraday Discussions, 2007, 134, 267-282.	1.6	151
6	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.	8.6	147
7	Why Are Polar Surfaces of ZnO Stable?. Chemistry of Materials, 2017, 29, 5306-5320.	3.2	141
8	Oxidation states and ionicity. Nature Materials, 2018, 17, 958-964.	13.3	135
9	Advances in computational studies of energy materials. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2010, 368, 3379-3456.	1.6	119
10	Polymorph Engineering of TiO₂: Demonstrating How Absolute Reference Potentials Are Determined by Local Coordination. Chemistry of Materials, 2015, 27, 3844-3851.	3.2	113
11	Structures of Zinc Oxide Nanoclusters: As Found by Revolutionary Algorithm Techniques. Journal of Physical Chemistry C, 2008, 112, 18860-18875.	1.5	106
12	Zinc oxide: A case study in contemporary computational solid state chemistry. Journal of Computational Chemistry, 2008, 29, 2234-2249.	1.5	105
13	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
14	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
15	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
16	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
17	Hole localization in [AlO4]0 defects in silica materials. Journal of Chemical Physics, 2005, 122, 144704.	1.2	74
18	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

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19	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
20	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
21	Electron Counting in Solids: Oxidation States, Partial Charges, and Ionicity. Journal of Physical Chemistry Letters, 2017, 8, 2074-2075.	2.1	65
22	Surface structure of zinc oxide (), using an atomistic, semi-infinite treatment. Surface Science, 2002, 498, 135-146.	0.8	64
23	Physical Properties, Intrinsic Defects, and Phase Stability of Indium Sesquioxide. Chemistry of Materials, 2009, 21, 4962-4969.	3.2	61
24	Limits to Doping of Wide Band Gap Semiconductors. Chemistry of Materials, 2013, 25, 2924-2926.	3.2	57
25	Microscopic origins of electron and hole stability in ZnO. Chemical Communications, 2011, 47, 3386.	2.2	54
26	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
27	True Structure of Trigonal Bipyramidal SiO4F-Species in Siliceous Zeolites. Chemistry of Materials, 2001, 13, 4708-4713.	3.2	52
28	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
29	Donor and acceptor characteristics of native point defects in GaN. Journal Physics D: Applied Physics, 2019, 52, 335104.	1.3	49
30	Oxygen interstitial structures in close-packed metal oxides. Chemical Physics Letters, 2010, 492, 44-48.	1.2	48
31	Dynamical response and instability in ceria under lattice expansion. Physical Review B, 2013, 87, .	1.1	48
32	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
33	QM/MM modelling of the TS-1 catalyst using HPCx. Journal of Materials Chemistry, 2006, 16, 1919.	6.7	45
34	Bubbles and microporous frameworks of silicon carbide. Physical Chemistry Chemical Physics, 2009, 11, 3186.	1.3	44
35	Electronic structure and magnetic coupling inFeSbO4: A DFT study using hybrid functionals andGGA+Umethods. Physical Review B, 2006, 73, .	1.1	43
36	Antiferromagnetism atT>500Kin the layered hexagonal ruthenateSrRu2O6. Physical Review B, 2015, 92, .	1.1	43

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37	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
38	Structure, optical properties and defects in nitride (IIIâ€“V) nanoscale cage clusters. Physical Chemistry Chemical Physics, 2008, 10, 1944.	1.3	42
39	Bulk electronic, elastic, structural, and dielectric properties of the Weyl semimetal TaAs. Physical Review B, 2016, 93, .	1.1	42
40	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
41	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
42	Embedded-cluster calculations in a numeric atomic orbital density-functional theory framework. Journal of Chemical Physics, 2014, 141, 024105.	1.2	38
43	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
44	The reactivity of CO₂on the MgO(100) surface. Physical Chemistry Chemical Physics, 2014, 16, 184-195.	1.3	36
45	Interlayer Cation Exchange Stabilizes Polar Perovskite Surfaces. Advanced Materials, 2014, 26, 7252-7256.	11.1	36
46	The nature of the oxidation states of gold on ZnO. Physical Chemistry Chemical Physics, 2005, 7, 2440.	1.3	35
47	An efficient genetic algorithm for structure prediction at the nanoscale. Nanoscale, 2017, 9, 3850-3864.	2.8	35
48	Construction of nano- and microporous frameworks from octahedral bubble clusters. Physical Chemistry Chemical Physics, 2009, 11, 3176.	1.3	34
49	Activation of Carbon Dioxide over Zinc Oxide by Localised Electrons. ChemPhysChem, 2012, 13, 3453-3456.	1.0	34
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	Bulk ionization potentials and band alignments from three-dimensional periodic calculations as demonstrated on rocksalt oxides. Physical Review B, 2014, 90, .	1.1	33
52	Morphological Features and Band Bending at Nonpolar Surfaces of ZnO. Journal of Physical Chemistry C, 2015, 119, 11598-11611.	1.5	33
53	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
54	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

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55	Adsorption of Organosilanes at a Zn-Terminated ZnO (0001) Surface:Â Molecular Dynamics Study. Langmuir, 2006, 22, 8036-8042.	1.6	30
56	On the problem of cluster structure diversity and the value of data mining. Physical Chemistry Chemical Physics, 2010, 12, 8438.	1.3	30
57	Potential energy landscapes for anion Frenkel-pair formation in ceria and india. Solid State Ionics, 2011, 184, 52-56.	1.3	29
58	Modelling metal centres, acid sites and reaction mechanisms in microporous catalysts. Faraday Discussions, 2016, 188, 235-255.	1.6	29
59	Understanding the interface between oxides and metals. Faraday Discussions, 2003, 124, 185.	1.6	28
60	Computational Investigation into the Origins of Lewis Acidity in Zeolites. Advanced Materials, 2000, 12, 1801-1805.	11.1	25
61	Formation of Heteroatom Active Sites in Zeolites by Hydrolysis and Inversion. Angewandte Chemie - International Edition, 2006, 45, 1633-1638.	7.2	25
62	Prediction of multiband luminescence due to the gallium vacancyâ€“oxygen defect complex in GaN. Applied Physics Letters, 2018, 112, .	1.5	25
63	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
64	Free energy of defect formation: Thermodynamics of anion Frenkel pairs in indium oxide. Physical Review B, 2011, 83, .	1.1	24
65	Formation of Active Sites in TS-1 by Hydrolysis and Inversion. Journal of Physical Chemistry C, 2007, 111, 14720-14731.	1.5	22
66	Prediction on the existence and chemical stability of cuprous fluoride. Chemical Science, 2012, 3, 2565.	3.7	22
67	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
68	Defect Centers in Microporous Aluminum Silicate Materials. Journal of Physical Chemistry B, 1998, 102, 10647-10649.	1.2	20
69	Nonstoichiometry and Weyl fermionic behavior in TaAs. Physical Review B, 2016, 94, .	1.1	20
70	Development of Interatomic Potentials for Supported Nanoparticles: The Cu/ZnO Case. Journal of Physical Chemistry C, 2017, 121, 16831-16844.	1.5	19
71	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
72	Thermodynamically accessible titanium clusters Ti_N, N = 2â€“32. Physical Chemistry Chemical Physics, 2018, 20, 13962-13973.	1.3	18

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73	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
74	Transformation of hydroxyl nests in microporous aluminosilicates upon annealing. Journal of Physics Condensed Matter, 2004, 16, S2781-S2794.	0.7	15
75	Defect structures in the silver halides. Physical Review B, 2008, 77, .	1.1	15
76	Active sites for heterogeneous catalysis by functionalisation of internal and external surfaces. Catalysis Today, 2004, 93-95, 535-540.	2.2	11
77	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
78	Electron and hole stability in GaN and ZnO. Journal of Physics Condensed Matter, 2011, 23, 334217.	0.7	11
79	Double bubbles: a new structural motif for enhanced electronâ€“hole separation in solids. Physical Chemistry Chemical Physics, 2014, 16, 21098-21105.	1.3	11
80	Modelling the chemistry of Mn-doped MgO for bulk and (100) surfaces. Physical Chemistry Chemical Physics, 2016, 18, 28648-28660.	1.3	11
81	From Ergodicity to Extended Phase Diagrams. Angewandte Chemie - International Edition, 2012, 51, 3752-3754.	7.2	10
82	From Stable ZnO and GaN Clusters to Novel Double Bubbles and Frameworks. Inorganics, 2014, 2, 248-263.	1.2	10
83	Hybrid-DFT Modeling of Lattice and Surface Vacancies in MnO. Journal of Physical Chemistry C, 2019, 123, 8133-8144.	1.5	10
84	From monomer to monolayer: a global optimisation study of (ZnO)_n nanoclusters on the Ag surface. Nanoscale, 2014, 6, 14754-14765.	2.8	9
85	Morphology of Cu clusters supported on reconstructed polar ZnO (0001) and (000Ì„) surfaces. Journal of Materials Chemistry A, 2020, 8, 22840-22857.	5.2	9
86	The reactivity of CO₂and H₂at trapped electron sites at an oxide surface. Physical Chemistry Chemical Physics, 2014, 16, 21153-21156.	1.3	8
87	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
88	Real and virtual polymorphism of titanium selenide with robust interatomic potentials. Journal of Materials Chemistry A, 2020, 8, 14054-14061.	5.2	8
89	Electron spin localisation and correlation effects for point defects in semi-ionic solids. Computational Materials Science, 2000, 17, 312-318.	1.4	7
90	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

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91	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
92	Materials and Molecular Modeling at the Exascale. Computing in Science and Engineering, 2022, 24, 36-45.	1.2	7
93	A model for the formation of point defects in zeolites. Radiation Effects and Defects in Solids, 1999, 151, 235-241.	0.4	6
94	One-dimensional embedded cluster approach to modeling CdS nanowires. Journal of Chemical Physics, 2013, 139, 124101.	1.2	6
95	BuckeridgeetÂal.Reply:. Physical Review Letters, 2015, 115, 029702.	2.9	6
96	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
97	Are octahedral clusters missing on the carbon energy landscape?. Nanoscale Advances, 2019, 1, 89-93.	2.2	6
98	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
99	Defect structures in silver chloride. Journal of Physics Condensed Matter, 2004, 16, S2827-S2838.	0.7	5
100	Magnetic properties of Fe2GeMo3N; an experimental and computational study. Journal of Materials Chemistry, 2012, 22, 15606.	6.7	5
101	Magnetic coupling constants for MnO as calculated using hybrid density functional theory. Chemical Physics Letters, 2017, 690, 47-53.	1.2	5
102	Semi-empirical supercell calculations for free- and bound-hole polarons in crystal. Journal of Physics Condensed Matter, 1997, 9, 3559-3573.	0.7	4
103	The initial stages of aminosilanol polymerisation. Chemical Communications, 2004, , 20.	2.2	4
104	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
105	The Interplay of Interstitial and Substitutional Copper in Zinc Oxide. Frontiers in Chemistry, 2021, 9, 780935.	1.8	4
106	25ÂÂComputer modelling of inorganic materials. Annual Reports on the Progress of Chemistry Section A, 2005, , .	0.8	3
107	A Computational Investigation of the Different Intermediates during Organoalkoxysilane Hydrolysis. Journal of Physical Chemistry B, 2006, 110, 24311-24317.	1.2	3
108	The RÃ1e of Defects in Photographic Latent Image Formation. Materials Research Society Symposia Proceedings, 2004, 848, 371.	0.1	2

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109	Modelling Structure and Defects in Zeolites. , 1997, , 125-135.		2
110	Computer Modelling of Catalysts and Catalysis. , 2000, , 3-60.		1
111	Applications of Density Functional Theory in Solid State Chemistry. ChemInform, 2003, 34, no.	0.1	1
112	From CO2 to Methanol by Hybrid QM/MM Embedding. , 2001, 40, 4437.		1
113	Zinc oxide: A case study in contemporary computational solid state chemistry. , 2008, 29, 2234.		1
114	Computer Modelling in Solid-State Chemistry. , 2007, , 180-207.		1
115	Understanding the interface between oxides and metals. , 0, .		1
116	Assignment of the complex vibrational spectra of the hydrogenated ZnO polar surfaces using QM/MM embedding. , 0, .		1
117	One-Dimensional Nanosystems. Series in Materials Science and Engineering, 2016, , 47-81.	0.1	1
118	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
119	Computational Approaches to the Determination of Active Site Structures and Reaction Mechanisms in Heterogeneous Catalysts. ChemInform, 2005, 36, no.	0.1	0