Alexey A Sokol

List of Publications by Citations

130 papers	6,159 citations	37 h-index	77 g-index
142 ext. papers	6,730 ext. citations	5.3 avg, IF	5.44 L-index

#	Paper	IF	Citations
130	Band alignment of rutile and anatase TiO. *Nature Materials*, **2013**, 12, 798-801	27	1656
129	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		790
128	ChemShell. modular software package for QM/MM simulations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 101-110	7.9	267
127	Modelling nano-clusters and nucleation. *Physical Chemistry Chemical Physics*, **2010**, 12, 786-811	3.6	160
126	Point defects in ZnO. *Faraday Discussions*, **2007**, 134, 267-82; discussion 315-29, 415-9	3.6	136
125	Advances in computational studies of energy materials. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2010**, 368, 3379-456	3	110
124	Anharmonicity in the High-Temperature Cmcm Phase of SnSe: Soft Modes and Three-Phonon Interactions. *Physical Review Letters*, **2016**, 117, 075502	7.4	104
123	Structures of Zinc Oxide Nanoclusters: As Found by Revolutionary Algorithm Techniques. *Journal of Physical Chemistry C*, **2008**, 112, 18860-18875	3.8	97
122	Zinc oxide: A case study in contemporary computational solid state chemistry. *Journal of Computational Chemistry*, **2008**, 29, 2234-49	3.5	95
121	Why Are Polar Surfaces of ZnO Stable?. *Chemistry of Materials*, **2017**, 29, 5306-5320	9.6	94
120	Polymorph Engineering of TiO2: Demonstrating How Absolute Reference Potentials Are Determined by Local Coordination. *Chemistry of Materials*, **2015**, 27, 3844-3851	9.6	92
119	Oxidation states and ionicity. *Nature Materials*, **2018**, 17, 958-964	27	91
118	From CO(2) 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*, **2004**, 43, 1127-1149	16.4	88
117	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, 913-36; discussion 1035-40	3	82
116	Hybrid QM/MM embedding approach for the treatment of localized surface states in ionic materials. *International Journal of Quantum Chemistry*, **2004**, 99, 695-712	2.1	82
115	Identification and Characterization of Active Sites and Their Catalytic Processes. the Cu/ZnO Methanol Catalyst. *Topics in Catalysis*, **2003**, 24, 161-172	2.3	79
114	Hole localization in [AlO4]0 defects in silica materials. *Journal of Chemical Physics*, **2005**, 122, 144704	3.9	68

113	Strontium migration assisted by oxygen vacancies in SrTiO3 from classical and quantum mechanical simulations. *Physical Review B*, **2011**, 83,	3.3	60
112	Physical Properties, Intrinsic Defects, and Phase Stability of Indium Sesquioxide. *Chemistry of Materials*, **2009**, 21, 4962-4969	9.6	59
111	Determination of the nitrogen vacancy as a shallow compensating center in GaN doped with divalent metals. *Physical Review Letters*, **2015**, 114, 016405	7.4	58
110	Surface structure of zinc oxide (101 0), using an atomistic, semi-infinite treatment. *Surface Science*, **2002**, 498, 135-146	1.8	57
109	Electron Counting in Solids: Oxidation States, Partial Charges, and Ionicity. *Journal of Physical Chemistry Letters*, **2017**, 8, 2074-2075	6.4	50
108	Microscopic origins of electron and hole stability in ZnO. *Chemical Communications*, **2011**, 47, 3386-8	5.8	50
107	True Structure of Trigonal Bipyramidal SiO4F- Species in Siliceous Zeolites. *Chemistry of Materials*, **2001**, 13, 4708-4713	9.6	50
106	Structure Prediction of Inorganic Nanoparticles with Predefined Architecture using a Genetic Algorithm. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2004**, 630, 2343-2353	1.3	49
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	3.4	47
104	From CO2 to Methanol by Hybrid QM/MM Embedding. *Angewandte Chemie*, **2001**, 113, 4569-4572	3.6	46
103	Deep vs shallow nature of oxygen vacancies and consequent n-type carrier concentrations in transparent conducting oxides. *Physical Review Materials*, **2018**, 2,	3.2	46
102	Limits to Doping of Wide Band Gap Semiconductors. *Chemistry of Materials*, **2013**, 25, 2924-2926	9.6	45
101	Oxygen interstitial structures in close-packed metal oxides. *Chemical Physics Letters*, **2010**, 492, 44-48	2.5	43
100	Bubbles and microporous frameworks of silicon carbide. *Physical Chemistry Chemical Physics*, **2009**, 11, 3186-200	3.6	42
99	QM/MM modelling of the TS-1 catalyst using HPCx. *Journal of Materials Chemistry*, **2006**, 16, 1919		42
98	Structure, optical properties and defects in nitride (III-V) nanoscale cage clusters. *Physical Chemistry Chemical Physics*, **2008**, 10, 1944-59	3.6	41
97	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	2.5	39
96	Dynamical response and instability in ceria under lattice expansion. *Physical Review B*, **2013**, 87,	3.3	38

95	Antiferromagnetism at T>500K in the layered hexagonal ruthenate SrRu2O6. *Physical Review B*, **2015**, 92,	3.3	38
94	Metal Cluster Support Interactions in the Cu/ZnO System: A QM/MM Study. *Journal of Physical Chemistry B*, **2003**, 107, 7045-7057	3.4	38
93	Electronic structure and magnetic coupling in FeSbO4: A DFT study using hybrid functionals and GGA+U methods. *Physical Review B*, **2006**, 73,	3.3	37
92	Interlayer cation exchange stabilizes polar perovskite surfaces. *Advanced Materials*, **2014**, 26, 7252-6	24	34
91	Bulk electronic, elastic, structural, and dielectric properties of the Weyl semimetal TaAs. *Physical Review B*, **2016**, 93,	3.3	33
90	Embedded-cluster calculations in a numeric atomic orbital density-functional theory framework. *Journal of Chemical Physics*, **2014**, 141, 024105	3.9	33
89	The nature of the oxidation states of gold on ZnO. *Physical Chemistry Chemical Physics*, **2005**, 7, 2440-5	3.6	33
88	Construction of nano- and microporous frameworks from octahedral bubble clusters. *Physical Chemistry Chemical Physics*, **2009**, 11, 3176-85	3.6	31
87	Structural and Optical Properties of Mg and Cd Doped ZnO Nanoclusters. *Journal of Physical Chemistry C*, **2013**, 117, 27127-27145	3.8	30
86	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	3.8	30
85	Assignment of the complex vibrational spectra of the hydrogenated ZnO polar surfaces using QM/MM embedding. *Journal of Chemical Physics*, **2003**, 118, 317-320	3.9	30
84	Donor and acceptor characteristics of native point defects in GaN. *Journal Physics D: Applied Physics* , **2019**, 52, 335104	3	28
83	Bulk ionization potentials and band alignments from three-dimensional periodic calculations as demonstrated on rocksalt oxides. *Physical Review B*, **2014**, 90,	3.3	28
82	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	3.9	28
81	Defect formation in In2O3 and SnO2: a new atomistic approach based on accurate lattice energies. *Journal of Materials Chemistry C*, **2018**, 6, 12386-12395	7.1	28
80	The reactivity of CO2 on the MgO(100) surface. *Physical Chemistry Chemical Physics*, **2014**, 16, 184-95	3.6	27
79	Morphological Features and Band Bending at Nonpolar Surfaces of ZnO. *Journal of Physical Chemistry C*, **2015**, 119, 11598-11611	3.8	27
78	An efficient genetic algorithm for structure prediction at the nanoscale. *Nanoscale*, **2017**, 9, 3850-3864	7.7	26

77	Modelling metal centres, acid sites and reaction mechanisms in microporous catalysts. *Faraday Discussions*, **2016**, 188, 235-55	3.6	26
76	Adsorption of organosilanes at a Zn-terminated ZnO (0001) surface: molecular dynamics study. *Langmuir*, **2006**, 22, 8036-42	4	26
75	Activation of carbon dioxide over zinc oxide by localised electrons. *ChemPhysChem*, **2012**, 13, 3453-6	3.2	25
74	On the problem of cluster structure diversity and the value of data mining. *Physical Chemistry Chemical Physics*, **2010**, 12, 8438-45	3.6	25
73	Understanding the interface between oxides and metals. *Faraday Discussions*, **2003**, 124, 185-203; discussion 205-13, 453-5	3.6	25
72	The Growth of Copper Clusters over ZnO: the Competition between Planar and Polyhedral Clusters. *Journal of Physical Chemistry C*, **2008**, 112, 7420-7430	3.8	24
71	Formation of heteroatom active sites in zeolites by hydrolysis and inversion. *Angewandte Chemie - International Edition*, **2006**, 45, 1633-8	16.4	23
70	Potential energy landscapes for anion Frenkel-pair formation in ceria and india. *Solid State Ionics*, **2011**, 184, 52-56	3.3	22
69	Prediction on the existence and chemical stability of cuprous fluoride. *Chemical Science*, **2012**, 3, 2565	9.4	21
68	Free energy of defect formation: Thermodynamics of anion Frenkel pairs in indium oxide. *Physical Review B*, **2011**, 83,	3.3	21
67	Formation of Active Sites in TS-1 by Hydrolysis and Inversion. *Journal of Physical Chemistry C*, **2007**, 111, 14720-14731	3.8	21
66	Computational Investigation into the Origins of Lewis Acidity in Zeolites. *Advanced Materials*, **2000**, 12, 1801-1805	24	19
65	Defect Centers in Microporous Aluminum Silicate Materials. *Journal of Physical Chemistry B*, **1998**, 102, 10647-10649	3.4	19
64	Development of Interatomic Potentials for Supported Nanoparticles: The Cu/ZnO Case. *Journal of Physical Chemistry C*, **2017**, 121, 16831-16844	3.8	17
63	Open-Source, Python-Based Redevelopment of the ChemShell Multiscale QM/MM Environment. *Journal of Chemical Theory and Computation*, **2019**, 15, 1317-1328	6.4	17
62	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	1.8	16
61	Nonstoichiometry and Weyl fermionic behavior in TaAs. *Physical Review B*, **2016**, 94,	3.3	16
60	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	2.4	15

59	Prediction of multiband luminescence due to the gallium vacancy–oxygen defect complex in GaN. *Applied Physics Letters*, **2018**, 112, 262104	3.4	15
58	Defect structures in the silver halides. *Physical Review B*, **2008**, 77,	3.3	12
57	Transformation of hydroxyl nests in microporous aluminosilicates upon annealing. *Journal of Physics Condensed Matter*, **2004**, 16, S2781-S2794	1.8	12
56	**2013**,		12
55	Electron and hole stability in GaN and ZnO. *Journal of Physics Condensed Matter*, **2011**, 23, 334217	1.8	11
54	Thermodynamically accessible titanium clusters Ti, N = 2-32. *Physical Chemistry Chemical Physics*, **2018**, 20, 13962-13973	3.6	10
53	Double bubbles: a new structural motif for enhanced electron-hole separation in solids. *Physical Chemistry Chemical Physics*, **2014**, 16, 21098-105	3.6	10
52	From Stable ZnO and GaN Clusters to Novel Double Bubbles and Frameworks. *Inorganics*, **2014**, 2, 248-263	2.9	10
51	Active sites for heterogeneous catalysis by functionalisation of internal and external surfaces. *Catalysis Today*, **2004**, 93-95, 535-540	5.3	10
50	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	1.6	9
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47	The reactivity of CO_2 and H_2 at trapped electron sites at an oxide surface. *Physical Chemistry Chemical Physics*, **2014**, 16, 21153-6	3.6	7
46	Ising-like antiferromagnetism on the octahedral sublattice of a cobalt-containing garnet and the potential for quantum criticality. *Physical Review B*, **2017**, 95,	3.3	7
45	Modelling the chemistry of Mn-doped MgO for bulk and (100) surfaces. *Physical Chemistry Chemical Physics*, **2016**, 18, 28648-28660	3.6	7
44	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	1.6	6
43	From ergodicity to extended phase diagrams. *Angewandte Chemie - International Edition*, **2012**, 51, 3752-4	16.4	6
42	One-dimensional embedded cluster approach to modeling CdS nanowires. *Journal of Chemical Physics*, **2013**, 139, 124101	3.9	6

41	Hybrid-DFT Modeling of Lattice and Surface Vacancies in MnO. *Journal of Physical Chemistry C*, **2019**, 123, 8133-8144	3.8	6
40	Are octahedral clusters missing on the carbon energy landscape?. *Nanoscale Advances*, **2019**, 1, 89-93	5.1	5
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38	Buckeridge et al. Reply. *Physical Review Letters*, **2015**, 115, 029702	7.4	5
37	Magnetic properties of Fe2GeMo3N; an experimental and computational study. *Journal of Materials Chemistry*, **2012**, 22, 15606		5
36	Electron spin localisation and correlation effects for point defects in semi-ionic solids. *Computational Materials Science*, **2000**, 17, 312-318	3.2	5
35	A model for the formation of point defects in zeolites. *Radiation Effects and Defects in Solids*, **1999**, 151, 235-241	0.9	5
34	Morphology of Cu clusters supported on reconstructed polar ZnO (0001) and (000) surfaces. *Journal of Materials Chemistry A*, **2020**, 8, 22840-22857	13	5
33	Real and virtual polymorphism of titanium selenide with robust interatomic potentials. *Journal of Materials Chemistry A*, **2020**, 8, 14054-14061	13	5
32	Magnetic coupling constants for MnO as calculated using hybrid density functional theory. *Chemical Physics Letters*, **2017**, 690, 47-53	2.5	4
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30	Semi-empirical supercell calculations for free- and bound-hole polarons in crystal. *Journal of Physics Condensed Matter*, **1997**, 9, 3559-3573	1.8	4
29	The initial stages of aminosilanol polymerisation. *Chemical Communications*, **2004**, 20-1	5.8	4
28	Energy Conversion: Solid Oxide Fuel Cells: First-Principles Modeling of Elementary Processes149-186		4
27	Computational Techniques **2013**, 1-28		3
26	Quantum Mechanical/Molecular Mechanical (QM/MM) Approaches **2017**, 647-680		3
25	25 Computer modelling of inorganic materials. *Annual Reports on the Progress of Chemistry Section A*, **2005**,		3
24	A computational investigation of the different intermediates during organoalkoxysilane hydrolysis. *Journal of Physical Chemistry B*, **2006**, 110, 24311-7	3.4	3

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22	Formation of Heteroatom Active Sites in Zeolites by Hydrolysis and Inversion. *Angewandte Chemie*, **2006**, 118, 1663-1668	3.6	2
21	The R□e of Defects in Photographic Latent Image Formation. *Materials Research Society Symposia Proceedings*, **2004**, 848, 371		2
20	Modelling Structure and Defects in Zeolites **1997**, 125-135		2
19	Energy Conversion: Solid-State Lighting231-259		2
18	Energy Generation: Solar Energy **2013**, 29-69		1
17	Vom Konzept lokaler Ergodizit□hin zu erweiterten Phasendiagrammen. *Angewandte Chemie*, **2012**, 124, 3814-3816	3.6	1
16	One-Dimensional Nanosystems. *Series in Materials Science and Engineering*, **2016**, 47-81		1
15	Chapter 11. Computer Modelling in Solid-State Chemistry **2007**, 180-207		1
14	Understanding the interface between oxides and metals		1
13	Assignment of the complex vibrational spectra of the hydrogenated ZnO polar surfaces using QM/MM embedding		1
12	Energy Conversion: Heterogeneous Catalysis187-229		1
11	A computational investigation of the adsorption of small copper clusters on the CeO(110) surface. *Physical Chemistry Chemical Physics*, **2021**, 23, 19329-19342	3.6	1
10	From CO2 to Methanol by Hybrid QM/MM Embedding **2001**, 40, 4437		1
9	Zinc oxide: A case study in contemporary computational solid state chemistry **2008**, 29, 2234		1
8	Materials and Molecular Modelling at the Exascale. *Computing in Science and Engineering*, **2022**, 1-1	1.5	0
7	The Interplay of Interstitial and Substitutional Copper in Zinc Oxide.. *Frontiers in Chemistry*, **2021**, 9, 780935		0
6	Energy Storage: Rechargeable Lithium Batteries **2013**, 109-129		

List of Publications

5 Energy Storage: Hydrogen **2013**, 131-148

4 Toward the Nanoscale **2013**, 261-294

3 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

2 Computer Modelling of Catalysts and Catalysis **2000**, 3-60

1 Energy Generation: Nuclear Energy71-107