Alexey A Sokol

List of Publications by Year in Descending Order

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	Materials and Molecular Modelling at the Exascale. *Computing in Science and Engineering*, **2022**, 1-1	1.5	0
129	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
128	The Interplay of Interstitial and Substitutional Copper in Zinc Oxide.. *Frontiers in Chemistry*, **2021**, 9, 780935	5	0
127	Morphology of Cu clusters supported on reconstructed polar ZnO (0001) and (000) surfaces. *Journal of Materials Chemistry A*, **2020**, 8, 22840-22857	13	5
126	Real and virtual polymorphism of titanium selenide with robust interatomic potentials. *Journal of Materials Chemistry A*, **2020**, 8, 14054-14061	13	5
125	Are octahedral clusters missing on the carbon energy landscape?. *Nanoscale Advances*, **2019**, 1, 89-93	5.1	5
124	Donor and acceptor characteristics of native point defects in GaN. *Journal Physics D: Applied Physics* , **2019**, 52, 335104	3	28
123	Hybrid-DFT Modeling of Lattice and Surface Vacancies in MnO. *Journal of Physical Chemistry C*, **2019** , 123, 8133-8144	3.8	6
122	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
121	Thermodynamically accessible titanium clusters Ti, N = 2-32. *Physical Chemistry Chemical Physics*, **2018**, 20, 13962-13973	3.6	10
120	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	3.6	5
119	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
118	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
117	Oxidation states and ionicity. *Nature Materials*, **2018**, 17, 958-964	27	91
116	Prediction of multiband luminescence due to the gallium vacancy–oxygen defect complex in GaN. *Applied Physics Letters*, **2018**, 112, 262104	3.4	15
115	An efficient genetic algorithm for structure prediction at the nanoscale. *Nanoscale*, **2017**, 9, 3850-3864	7.7	26
114	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

113	Why Are Polar Surfaces of ZnO Stable?. *Chemistry of Materials*, **2017**, 29, 5306-5320	9.6	94
112	Electron Counting in Solids: Oxidation States, Partial Charges, and Ionicity. *Journal of Physical Chemistry Letters*, **2017**, 8, 2074-2075	6.4	50
111	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
110	Magnetic coupling constants for MnO as calculated using hybrid density functional theory. *Chemical Physics Letters*, **2017**, 690, 47-53	2.5	4
109	Quantum Mechanical/Molecular Mechanical (QM/MM) Approaches **2017**, 647-680		3
108	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
107	Development of Interatomic Potentials for Supported Nanoparticles: The Cu/ZnO Case. *Journal of Physical Chemistry C*, **2017**, 121, 16831-16844	3.8	17
106	Anharmonicity in the High-Temperature Cmcm Phase of SnSe: Soft Modes and Three-Phonon Interactions. *Physical Review Letters*, **2016**, 117, 075502	7.4	104
105	Modelling metal centres, acid sites and reaction mechanisms in microporous catalysts. *Faraday Discussions*, **2016**, 188, 235-55	3.6	26
104	Bulk electronic, elastic, structural, and dielectric properties of the Weyl semimetal TaAs. *Physical Review B*, **2016**, 93,	3.3	33
103	Double bubble secondary building units used as a structural motif for enhanced electron□hole separation in solids. *Materials Science in Semiconductor Processing*, **2016**, 42, 147-149	4.3	4
102	One-Dimensional Nanosystems. *Series in Materials Science and Engineering*, **2016**, 47-81		1
101	Nonstoichiometry and Weyl fermionic behavior in TaAs. *Physical Review B*, **2016**, 94,	3.3	16
100	Modelling the chemistry of Mn-doped MgO for bulk and (100) surfaces. *Physical Chemistry Chemical Physics*, **2016**, 18, 28648-28660	3.6	7
99	Polymorph Engineering of TiO2: Demonstrating How Absolute Reference Potentials Are Determined by Local Coordination. *Chemistry of Materials*, **2015**, 27, 3844-3851	9.6	92
98	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
97	Antiferromagnetism at T>500K in the layered hexagonal ruthenate SrRu2O6. *Physical Review B*, **2015**, 92,	3.3	38
96	Buckeridge et□al. Reply. *Physical Review Letters*, **2015**, 115, 029702	7.4	5

95	Morphological Features and Band Bending at Nonpolar Surfaces of ZnO. *Journal of Physical Chemistry C*, **2015**, 119, 11598-11611	3.8	27
94	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
93	ChemShell□ modular software package for QM/MM simulations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 101-110	7.9	267
92	From monomer to monolayer: a global optimisation study of (ZnO)n nanoclusters on the Ag surface. *Nanoscale*, **2014**, 6, 14754-65	7.7	8
91	Double bubbles: a new structural motif for enhanced electron-hole separation in solids. *Physical Chemistry Chemical Physics*, **2014**, 16, 21098-105	3.6	10
90	The reactivity of CO□and H□at trapped electron sites at an oxide surface. *Physical Chemistry Chemical Physics*, **2014**, 16, 21153-6	3.6	7
89	The reactivity of CO2 on the MgO(100) surface. *Physical Chemistry Chemical Physics*, **2014**, 16, 184-95	3.6	27
88	Bulk ionization potentials and band alignments from three-dimensional periodic calculations as demonstrated on rocksalt oxides. *Physical Review B*, **2014**, 90,	3.3	28
87	Interlayer cation exchange stabilizes polar perovskite surfaces. *Advanced Materials*, **2014**, 26, 7252-6	24	34
86	From Stable ZnO and GaN Clusters to Novel Double Bubbles and Frameworks. *Inorganics*, **2014**, 2, 248-263	3.9	10
85	Embedded-cluster calculations in a numeric atomic orbital density-functional theory framework. *Journal of Chemical Physics*, **2014**, 141, 024105	3.9	33
84	Limits to Doping of Wide Band Gap Semiconductors. *Chemistry of Materials*, **2013**, 25, 2924-2926	9.6	45
83	Band alignment of rutile and anatase TiO□*Nature Materials*, **2013**, 12, 798-801	27	1656
82	Dynamical response and instability in ceria under lattice expansion. *Physical Review B*, **2013**, 87,	3.3	38
81	Energy Storage: Rechargeable Lithium Batteries **2013**, 109-129		
80	Structural and Optical Properties of Mg and Cd Doped ZnO Nanoclusters. *Journal of Physical Chemistry C*, **2013**, 117, 27127-27145	3.8	30
79	Computational Techniques **2013**, 1-28		3
78	Energy Generation: Solar Energy **2013**, 29-69		1

77	Energy Storage: Hydrogen **2013**, 131-148		
76	Toward the Nanoscale **2013**, 261-294		
75	One-dimensional embedded cluster approach to modeling CdS nanowires. *Journal of Chemical Physics*, **2013**, 139, 124101	3.9	6
74	**2013**,		12
73	Magnetic properties of Fe2GeMo3N; an experimental and computational study. *Journal of Materials Chemistry*, **2012**, 22, 15606		5
72	Prediction on the existence and chemical stability of cuprous fluoride. *Chemical Science*, **2012**, 3, 2565	9.4	21
71	Vom Konzept lokaler Ergodizität hin zu erweiterten Phasendiagrammen. *Angewandte Chemie*, **2012**, 124, 3814-3816	3.6	1
70	From ergodicity to extended phase diagrams. *Angewandte Chemie - International Edition*, **2012**, 51, 3752-56	6.4	6
69	Activation of carbon dioxide over zinc oxide by localised electrons. *ChemPhysChem*, **2012**, 13, 3453-6	3.2	25
68	Electron and hole stability in GaN and ZnO. *Journal of Physics Condensed Matter*, **2011**, 23, 334217	1.8	11
67	Microscopic origins of electron and hole stability in ZnO. *Chemical Communications*, **2011**, 47, 3386-8	5.8	50
66	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
65	Potential energy landscapes for anion Frenkel-pair formation in ceria and india. *Solid State Ionics*, **2011**, 184, 52-56	3.3	22
64	Strontium migration assisted by oxygen vacancies in SrTiO3 from classical and quantum mechanical simulations. *Physical Review B*, **2011**, 83,	3.3	60
63	Free energy of defect formation: Thermodynamics of anion Frenkel pairs in indium oxide. *Physical Review B*, **2011**, 83,	3.3	21
62	Modelling nano-clusters and nucleation. *Physical Chemistry Chemical Physics*, **2010**, 12, 786-811	3.6	160
61	On the problem of cluster structure diversity and the value of data mining. *Physical Chemistry Chemical Physics*, **2010**, 12, 8438-45	3.6	25
60	Advances in computational studies of energy materials. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2010**, 368, 3379-456	3	110

59	Oxygen interstitial structures in close-packed metal oxides. *Chemical Physics Letters*, **2010**, 492, 44-48	2.5	43
58	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
57	Physical Properties, Intrinsic Defects, and Phase Stability of Indium Sesquioxide. *Chemistry of Materials*, **2009**, 21, 4962-4969	9.6	59
56	Construction of nano- and microporous frameworks from octahedral bubble clusters. *Physical Chemistry Chemical Physics*, **2009**, 11, 3176-85	3.6	31
55	Bubbles and microporous frameworks of silicon carbide. *Physical Chemistry Chemical Physics*, **2009**, 11, 3186-200	3.6	42
54	Structures of Zinc Oxide Nanoclusters: As Found by Revolutionary Algorithm Techniques. *Journal of Physical Chemistry C*, **2008**, 112, 18860-18875	3.8	97
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	3.8	30
52	Structure, optical properties and defects in nitride (III-V) nanoscale cage clusters. *Physical Chemistry Chemical Physics*, **2008**, 10, 1944-59	3.6	41
51	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
50	Defect structures in the silver halides. *Physical Review B*, **2008**, 77,	3.3	12
49	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	3.9	8
48	Zinc oxide: A case study in contemporary computational solid state chemistry. *Journal of Computational Chemistry*, **2008**, 29, 2234-49	3.5	95
47	Zinc oxide: A case study in contemporary computational solid state chemistry **2008**, 29, 2234		1
46	Formation of Active Sites in TS-1 by Hydrolysis and Inversion. *Journal of Physical Chemistry C*, **2007**, 111, 14720-14731	3.8	21
45	Point defects in ZnO. *Faraday Discussions*, **2007**, 134, 267-82; discussion 315-29, 415-9	3.6	136
44	Chapter 11. Computer Modelling in Solid-State Chemistry **2007**, 180-207		1
43	Formation of heteroatom active sites in zeolites by hydrolysis and inversion. *Angewandte Chemie - International Edition*, **2006**, 45, 1633-8	16.4	23
42	Formation of Heteroatom Active Sites in Zeolites by Hydrolysis and Inversion. *Angewandte Chemie*, **2006**, 118, 1663-1668	3.6	2

41	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
40	Adsorption of organosilanes at a Zn-terminated ZnO (0001) surface: molecular dynamics study. *Langmuir*, **2006**, 22, 8036-42	4	26
39	QM/MM modelling of the TS-1 catalyst using HPCx. *Journal of Materials Chemistry*, **2006**, 16, 1919		42
38	A computational investigation of the different intermediates during organoalkoxysilane hydrolysis. *Journal of Physical Chemistry B*, **2006**, 110, 24311-7	3.4	3
37	Hole localization in [AlO4]0 defects in silica materials. *Journal of Chemical Physics*, **2005**, 122, 144704	3.9	68
36	25 Computer modelling of inorganic materials. *Annual Reports on the Progress of Chemistry Section A*, **2005**,		3
35	The nature of the oxidation states of gold on ZnO. *Physical Chemistry Chemical Physics*, **2005**, 7, 2440-5	3.6	33
34	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
33	Transformation of hydroxyl nests in microporous aluminosilicates upon annealing. *Journal of Physics Condensed Matter*, **2004**, 16, S2781-S2794	1.8	12
32	Defect structures in silver chloride. *Journal of Physics Condensed Matter*, **2004**, 16, S2827-S2838	1.8	3
31	The Rle of Defects in Photographic Latent Image Formation. *Materials Research Society Symposia Proceedings*, **2004**, 848, 371		2
30	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
29	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
28	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
27	Active sites for heterogeneous catalysis by functionalisation of internal and external surfaces. *Catalysis Today*, **2004**, 93-95, 535-540	5.3	10
26	The initial stages of aminosilanol polymerisation. *Chemical Communications*, **2004**, 20-1	5.8	4
25	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
24	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

23	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
22	Understanding the interface between oxides and metals. *Faraday Discussions*, **2003**, 124, 185-203; discussion 205-13, 453-5	3.6	25
21	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
20	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
19	Surface structure of zinc oxide (101 0), using an atomistic, semi-infinite treatment. *Surface Science*, **2002**, 498, 135-146	1.8	57
18	From CO2 to Methanol by Hybrid QM/MM Embedding. *Angewandte Chemie*, **2001**, 113, 4569-4572	3.6	46
17	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*, **2001**, 40, 4437-4440	16.4	88
16	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		
15	True Structure of Trigonal Bipyramidal SiO4F- Species in Siliceous Zeolites. *Chemistry of Materials*, **2001**, 13, 4708-4713	9.6	50
14	From CO2 to Methanol by Hybrid QM/MM Embedding **2001**, 40, 4437		1
13	Computational Investigation into the Origins of Lewis Acidity in Zeolites. *Advanced Materials*, **2000**, 12, 1801-1805	24	19
12	Electron spin localisation and correlation effects for point defects in semi-ionic solids. *Computational Materials Science*, **2000**, 17, 312-318	3.2	5
11	Computer Modelling of Catalysts and Catalysis **2000**, 3-60		
10	A model for the formation of point defects in zeolites. *Radiation Effects and Defects in Solids*, **1999**, 151, 235-241	0.9	5
9	Defect Centers in Microporous Aluminum Silicate Materials. *Journal of Physical Chemistry B*, **1998**, 102, 10647-10649	3.4	19
8	Semi-empirical supercell calculations for free- and bound-hole polarons in crystal. *Journal of Physics Condensed Matter*, **1997**, 9, 3559-3573	1.8	4
7	Modelling Structure and Defects in Zeolites **1997**, 125-135		2
6	Understanding the interface between oxides and metals		1

List of Publications

5	Assignment of the complex vibrational spectra of the hydrogenated ZnO polar surfaces using QM/MM embedding	1
4	Energy Conversion: Heterogeneous Catalysis187-229	1
3	Energy Generation: Nuclear Energy71-107	
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1	Energy Conversion: Solid-State Lighting231-259	2