Stefan Bromley

List of Publications by Year
in descending order

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176 papers	7,069 citations	61945 43 h-index	69214 77 g-index
185 all docs	185 docs citations	185 times ranked	7185 citing authors

#	Article	IF	Citations
1	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
2	Correlation between Crystal Structure and Mobility in Organic Field-Effect Transistors Based on Single Crystals of Tetrathiafulvalene Derivatives. Journal of the American Chemical Society, 2004, 126, 8546-8553.	6.6	265
3	Dramatic reduction of the oxygen vacancy formation energy in ceria particles: a possible key to their remarkable reactivity at the nanoscale. Journal of Materials Chemistry, 2010, 20, 10535.	6.7	192
4	Modelling nano-clusters and nucleation. Physical Chemistry Chemical Physics, 2010, 12, 786-811.	1.3	174
5	Importance of Intermolecular Interactions in Assessing Hopping Mobilities in Organic Field Effect Transistors:Â Pentacene versus Dithiophene-tetrathiafulvalene. Journal of the American Chemical Society, 2004, 126, 6544-6545.	6.6	161
6	Greatly facilitated oxygen vacancy formation in ceria nanocrystallites. Chemical Communications, 2010, 46, 5936.	2.2	160
7	Point defects in ZnO. Faraday Discussions, 2007, 134, 267-282.	1.6	151
8	Dust formation in the oxygen-rich AGB star IK Tauri. Astronomy and Astrophysics, 2016, 585, A6.	2.1	141
9	Single-crystal organic field-effect transistors based on dibenzo-tetrathiafulvalene. Applied Physics Letters, 2005, 86, 012110.	1.5	130
10	Density functional studies of model cerium oxide nanoparticles. Physical Chemistry Chemical Physics, 2008, 10, 5730.	1.3	125
11	Preparation and characterisation of a highly active bimetallic (Pdâ€“Ru) nanoparticle heterogeneous catalystâ€. Chemical Communications, 1999, , 1571-1572.	2.2	124
12	Ultralow-Density Nanocage-Based Metal-Oxide Polymorphs. Physical Review Letters, 2007, 99, 235502.	2.9	119
13	Kondo Effect in a Neutral and Stable All Organic Radical Single Molecule Break Junction. Nano Letters, 2015, 15, 3109-3114.	4.5	117
14	Formation of Superoxide Anions on Ceria Nanoparticles by Interaction of Molecular Oxygen with Ce³⁺ Sites. Journal of Physical Chemistry C, 2011, 115, 5817-5822.	1.5	107
15	Approaching nanoscale oxides: models and theoretical methods. Chemical Society Reviews, 2009, 38, 2657.	18.7	105
16	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
17	Understanding Ceria Nanoparticles from First-Principles Calculations. Journal of Physical Chemistry C, 2007, 111, 10142-10145.	1.5	99
18	A new interatomic potential for nanoscale silica. Chemical Physics Letters, 2003, 378, 622-629.	1.2	98

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19	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
20	Fully Coordinated Silica Nanoclusters:(SiO2)NMolecular Rings. Physical Review Letters, 2003, 90, 035502.	2.9	94
21	Dedicated Global Optimization Search for Ground State Silica Nanoclusters:â€‰ (SiO2)N (N = 6â˜12). Journal of Physical Chemistry B, 2004, 108, 9638-9645.	1.2	88
22	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
23	When Anatase Nanoparticles Become Bulklike: Properties of Realistic TiO₂ Nanoparticles in the 1â€“6 nm Size Range from All Electron Relativistic Density Functional Theory Based Calculations. Journal of Chemical Theory and Computation, 2017, 13, 1785-1793.	2.3	87
24	Predicting size-dependent emergence of crystallinity in nanomaterials: titania nanoclusters versus nanocrystals. Nanoscale, 2017, 9, 1049-1058.	2.8	79
25	Size-Dependent Level Alignment between Rutile and Anatase TiO₂ Nanoparticles: Implications for Photocatalysis. Journal of Physical Chemistry Letters, 2017, 8, 5593-5598.	2.1	75
26	Theoretical Investigation of the Hydrogenation of (TiO₂)_NClusters (N= 1â€“10). Journal of Physical Chemistry C, 2011, 115, 15890-15899.	1.5	69
27	Exchange Coupling Inversion in a High-Spin Organic Triradical Molecule. Nano Letters, 2016, 16, 2066-2071.	4.5	60
28	Room Temperature Methane Capture and Activation by Ni Clusters Supported on TiC(001): Effects of Metalâ€“Carbide Interactions on the Cleavage of the Câ€“H Bond. Journal of the American Chemical Society, 2019, 141, 5303-5313.	6.6	57
29	New insights into the structure of supported bimetallic nanocluster catalysts prepared from carbonylated precursors: a combined density functional theory and EXAFS study. Chemical Physics Letters, 2001, 340, 524-530.	1.2	55
30	Thermodynamic limits on hydrogen storage in sodalite framework materials: a molecular mechanics investigation. Microporous and Mesoporous Materials, 2005, 78, 63-71.	2.2	55
31	Effect of Size and Structure on the Ground-State and Excited-State Electronic Structure of TiO₂ Nanoparticles. Journal of Chemical Theory and Computation, 2016, 12, 3751-3763.	2.3	53
32	Thermodynamic Stability of Discrete Fully Coordinated SiO2 Spherical and Elongated Nanocages. Nano Letters, 2004, 4, 1427-1432.	4.5	51
33	Exploring Ce3+/Ce4+ cation ordering in reduced ceria nanoparticles using interionic-potential and density-functional calculations. Journal of Chemical Physics, 2009, 131, 064701.	1.2	50
34	Tuning Crystal Ordering, Electronic Structure, and Morphology in Organic Semiconductors: Tetrathiafulvalenes as a Model Case. Advanced Functional Materials, 2016, 26, 2256-2275.	7.8	50
35	Columnar-to-Disk Structural Transition in Nanoscale(SiO2)NClusters. Physical Review Letters, 2005, 95, 185505.	2.9	49
36	Size dependent structural and polymorphic transitions in ZnO: from nanocluster to bulk. Nanoscale, 2017, 9, 10067-10074.	2.8	49

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37	Toward Understanding the Thermodynamic Viability of Zeolites and Related Frameworks through a Simple Topological Model. Chemistry of Materials, 2004, 16, 3809-3820.	3.2	48
38	Toward Understanding Extra-Large-Pore Zeolite Energetics and Topology:â€‰ A Polyhedral Approach. Chemistry of Materials, 2004, 16, 12-20.	3.2	47
39	Apparent Scarcity of Low-Density Polymorphs of Inorganic Solids. Physical Review Letters, 2010, 104, 175503.	2.9	46
40	Dramatic Influence of the Electronic Structure on the Conductivity through Openâ€•and Closedâ€Shell Molecules. Advanced Materials, 2009, 21, 1177-1181.	11.1	45
41	An extensive theoretical survey of low-density allotropy in silicon. Physical Chemistry Chemical Physics, 2010, 12, 8505.	1.3	45
42	Existence of multi-radical and closed-shell semiconducting states in post-graphene organic Dirac materials. Nature Communications, 2017, 8, 1957.	5.8	45
43	Understanding the interplay between size, morphology and energy gap in photoactive TiO₂nanoparticles. Nanoscale, 2019, 11, 9032-9041.	2.8	45
44	Diffusion of Molecular Hydrogen through Porous Materials:â€‰ The Importance of Framework Flexibility. Journal of Physical Chemistry B, 2004, 108, 5088-5094.	1.2	44
45	Dependence of charge transfer reorganization energy on carrier localisation in organic molecular crystals. Physical Chemistry Chemical Physics, 2008, 10, 121-127.	1.3	43
46	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
47	Development of realistic models for Double Metal Cyanide catalyst active sites. Journal of Molecular Modeling, 2007, 13, 751-756.	0.8	42
48	Prediction of half-metallic conductivity in Prussian Blue derivatives. Journal of Materials Chemistry, 2009, 19, 2032.	6.7	41
49	Structural and electronic bistability in ZnS single sheets and single-walled nanotubes. Physical Review B, 2011, 83, .	1.1	41
50	Electronic, Structural and Functional Versatility in Tetrathiafulvaleneâ€Lanthanide Metalâ€“Organic Frameworks. Chemistry - A European Journal, 2019, 25, 12636-12643.	1.7	40
51	Molecular-dynamics analysis of the diffusion of molecular hydrogen in all-silica sodalite. Journal of Chemical Physics, 2004, 120, 10285-10289.	1.2	38
52	Band Gap Variation in Prussian Blue via Cation-Induced Structural Distortion. Journal of Physical Chemistry B, 2006, 110, 24294-24298.	1.2	37
53	Adsorption isotherms of H2 in microporous materials with the SOD structure: A grand canonical Monte Carlo study. Microporous and Mesoporous Materials, 2006, 87, 235-242.	2.2	37
54	Under what conditions does (SiO)_N nucleation occur? A bottom-up kinetic modelling evaluation. Physical Chemistry Chemical Physics, 2016, 18, 26913-26922.	1.3	37

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55	Assessing the usefulness of transition metal carbides for hydrogenation reactions. Chemical Communications, 2019, 55, 12797-12800.	2.2	37
56	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
57	Dust in brown dwarfs and extra-solar planets. Astronomy and Astrophysics, 2015, 575, A11.	2.1	36
58	On the prediction of the crystal and electronic structure of mixed-valence materials by periodic density functional calculations: The case of Prussian Blue. Journal of Chemical Physics, 2008, 128, 044713.	1.2	35
59	Understanding the nature and location of hydroxyl groups on hydrated titania nanoparticles. Nanoscale, 2021, 13, 6577-6585.	2.8	35
60	Efficient nucleation of stardust silicates via heteromolecular homogeneous condensation. Monthly Notices of the Royal Astronomical Society, 2012, , no-no.	1.6	33
61	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
62	Nucleation of Small Silicon Carbide Dust Clusters in AGB Stars. Astrophysical Journal, 2017, 840, 117.	1.6	32
63	Factors Affecting Ionicity in All-Silica Materials:Â A Density Functional Cluster Study. Journal of Physical Chemistry A, 2002, 106, 12376-12385.	1.1	31
64	Stable nanoporous alkali halide polymorphs: a first principles bottom-up study. Journal of Materials Chemistry, 2008, 18, 5871.	6.7	30
65	Negative differential resistance (NDR) in similar molecules with distinct redox behaviour. Chemical Communications, 2011, 47, 4664.	2.2	30
66	Structure and Properties of Nanosilicates with Olivine (Mg₂SiO₄)_N and Pyroxene (MgSiO₃)_N Compositions. ACS Earth and Space Chemistry, 2019, 3, 2390-2403.	1.2	30
67	Understanding the interface between oxides and metals. Faraday Discussions, 2003, 124, 185.	1.6	28
68	Magic Silica Clusters as Nanoscale Building Units for Super-(Tris)tetrahedral Materials. Chemistry of Materials, 2006, 18, 1464-1469.	3.2	27
69	Hydrogen and oxygen adsorption on a nanosilicate - a quantum chemical study. Monthly Notices of the Royal Astronomical Society, 2011, 414, 1285-1291.	1.6	27
70	Molecular modelling of the transport behaviour of C3 and C4 gases through the zeolite DD3R. Microporous and Mesoporous Materials, 2002, 53, 45-57.	2.2	26
71	Predicting transition pressures for obtaining nanoporous semiconductor polymorphs: oxides and chalcogenides of Zn, Cd and Mg. Physical Chemistry Chemical Physics, 2010, 12, 8513.	1.3	26
72	Bandgap engineering through nanoporosity. Nanoscale, 2014, 6, 1181-1187.	2.8	26

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73	Challenges in modelling the reaction chemistry of interstellar dust. Physical Chemistry Chemical Physics, 2014, 16, 18623.	1.3	26
74	Computational insights into the role of Ge in stabilising double-four ring containing zeolites. Microporous and Mesoporous Materials, 2004, 73, 171-174.	2.2	25
75	Octahedrality versus tetrahedrality in stoichiometric ceria nanoparticles. Chemical Communications, 2012, 48, 4199.	2.2	25
76	Operative Mechanism of Hole-Assisted Negative Charge Motion in Ground States of Radical-Anion Molecular Wires. Journal of the American Chemical Society, 2017, 139, 686-692.	6.6	25
77	Structural richness of ionic binary materials: An exploration of the energy landscape of magnesium oxide. Physical Review B, 2011, 83, .	1.1	24
78	Nanofilm versus Bulk Polymorphism in Wurtzite Materials. Physical Review Letters, 2013, 110, 245501.	2.9	24
79	Efficient calculation of the structural and electronic properties of mixed valence materials: application to Prussian Blue analogues. Chemical Physics Letters, 2004, 397, 154-159.	1.2	23
80	Interaction of SiO2with Single-Walled Carbon Nanotubes. Journal of Physical Chemistry B, 2005, 109, 1387-1391.	1.2	23
81	Persistence of magic cluster stability in ultra-thin semiconductor nanorods. Nanoscale, 2010, 2, 72-77.	2.8	23
82	Enhancing Longâ€Term Device Stability Using Thin Film Blends of Small Molecule Semiconductors and Insulating Polymers to Trap Surfaceâ€Induced Polymorphs. Advanced Functional Materials, 2020, 30, 2006115.	7.8	23
83	Molecular hydrogen confined within nanoporous framework materials: Comparison of density functional and classical force-field descriptions. Physical Review B, 2005, 72, .	1.1	22
84	Chiral Conformation at a Molecular Level of a Propeller-Like Open-Shell Molecule on Au(111). Journal of Physical Chemistry Letters, 2012, 3, 1559-1564.	2.1	22
85	Perspectives for polychlorinated trityl radicals. Journal of Materials Chemistry C, 2021, 9, 10610-10623.	2.7	22
86	Bottom-up dust nucleation theory in oxygen-rich evolved stars. Astronomy and Astrophysics, 2022, 658, A167.	2.1	22
87	Energetics and structures of the initial stages of nucleation of (SiO2)Nspecies: possible routes to highly symmetrical tetrahedral clusters. Physical Chemistry Chemical Physics, 2007, 9, 1078-1086.	1.3	21
88	Competing mechanisms of catalytic H2 formation and dissociation on ultrasmall silicate nanocluster dust grains. Monthly Notices of the Royal Astronomical Society, 2013, 435, 1486-1492.	1.6	21
89	Low reactivity of non-bridging oxygen defects on stoichiometric silica surfaces. Chemical Communications, 2008, , 4156.	2.2	20
90	Reduced ceria nanofilms from structure prediction. Nanoscale, 2015, 7, 4361-4366.	2.8	20

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91	Importance of the embedding environment on the strain within small rings in siliceous materials. Physical Review B, 2006, 73, .	1.1	19
92	Stardust silicate nucleation kick-started by SiO+TiO ₂. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2013, 371, 20110580.	1.6	19
93	Development of Interatomic Potentials for Supported Nanoparticles: The Cu/ZnO Case. Journal of Physical Chemistry C, 2017, 121, 16831-16844.	1.5	19
94	Two-ring vibrational modes on silica surfaces investigated via fully coordinated nanoclusters. Surface Science, 2003, 539, L554-L559.	0.8	18
95	Bromleyet al.Reply:. Physical Review Letters, 2004, 92, .	2.9	18
96	Effect of cation distribution on self-diffusion of molecular hydrogen in Na3Al3Si3O12 sodalite:â€‚A molecular dynamics study. Journal of Chemical Physics, 2004, 121, 10209-10216.	1.2	18
97	New materials from fully coordinated SiO2 nanoclusters. Computational Materials Science, 2006, 35, 382-386.	1.4	18
98	The fate of optical excitations in small hydrated ZnS clusters: a theoretical study into the effect of hydration on the excitation and localisation of electrons in Zn4S4 and Zn6S6. Physical Chemistry Chemical Physics, 2011, 13, 9311.	1.3	18
99	The fate of optical excitations in small polyhedral ZnS clusters: A theoretical study of the excitation and localization of electrons in Zn4S4and Zn6S6. Journal of Chemical Physics, 2011, 134, 064511.	1.2	18
100	A global optimisation study of the low-lying isomers of the alumina octomer (Al2O3)8. Chemical Physics Letters, 2018, 711, 138-147.	1.2	18
101	What Can Infrared Spectra Tell Us about the Crystallinity of Nanosized Interstellar Silicate Dust Grains?. ACS Earth and Space Chemistry, 2019, 3, 2323-2338.	1.2	18
102	Controlling pairing of Ï€-conjugated electrons in 2D covalent organic radical frameworks via in-plane strain. Nature Communications, 2021, 12, 1705.	5.8	18
103	Defective to fully coordinated crossover in complex directionally bonded nanoclusters. Physical Review B, 2009, 80, .	1.1	17
104	Prospective Role of Multicenter Bonding for Efficient and Selective Hydrogen Transport. Physical Review Letters, 2010, 105, 045901.	2.9	17
105	Diversity of Adsorbed Hydrogen on the TiC(001) Surface at High Coverages. Journal of Physical Chemistry C, 2018, 122, 28013-28020.	1.5	17
106	Bimetallic clusters supported on mesoporous silica: the effects of support interactions on cluster morphology. Microporous and Mesoporous Materials, 2001, 44-45, 395-399.	2.2	16
107	Novel structures and energy spectra of hydroxylated (SiO2)8-based clusters: Searching for the magic (SiO2)8O2H3â^' cluster. Journal of Chemical Physics, 2005, 122, 114303.	1.2	16
108	Design of multi-functional 2D open-shell organic networks with mechanically controllable properties. Chemical Science, 2017, 8, 1027-1039.	3.7	16

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109	Stability of mixed-oxide titanosilicates: dependency on size and composition from nanocluster to bulk. Nanoscale, 2018, 10, 832-842.	2.8	16
110	Prospects for a synthetic route towards well-defined stoichiometric silica nanoclusters: from siloxane to silica. Chemical Physics Letters, 2004, 385, 389-393.	1.2	15
111	Modelling organic molecular crystals by hybrid quantum mechanical/molecular mechanical embedding. Chemical Physics Letters, 2008, 457, 154-158.	1.2	15
112	Hydroxylation of silica nanoclusters (SiO2)M(H2O)N, M = 4, 8, 16, 24: stability and structural trends. Physical Chemistry Chemical Physics, 2013, 15, 20438.	1.3	15
113	Structural control over spin localization in triarylmethyls. RSC Advances, 2015, 5, 98593-98599.	1.7	15
114	Structure direction in zinc oxide and related materials by cation substitution: an analogy with zeolites. Journal of Materials Chemistry, 2011, 21, 15255.	6.7	14
115	HOMO Stabilisation in Ï€â€Extended Dibenzotetrathiafulvalene Derivatives for Their Application in Organic Fieldâ€Effect Transistors. Chemistry - A European Journal, 2014, 20, 16672-16679.	1.7	14
116	Global optimisation of hydroxylated silica clusters: A cascade Monte Carlo Basin Hopping approach. Computational and Theoretical Chemistry, 2017, 1102, 38-43.	1.1	14
117	How hydroxylation affects hydrogen adsorption and formation on nanosilicates. Molecular Astrophysics, 2017, 7, 1-8.	1.7	14
118	2D Hexagonal Covalent Organic Radical Frameworks as Tunable Correlated Electron Systems. Advanced Functional Materials, 2021, 31, 2004584.	7.8	14
119	Evidence for atomic mixingvia multiple intermediates during the dynamic interconversion of silicate oligomers in solution. Chemical Communications, 2012, 48, 46-48.	2.2	13
120	Trends in the adsorption and reactivity of hydrogen on magnesium silicate nanoclusters. Physical Chemistry Chemical Physics, 2015, 17, 8951-8963.	1.3	13
121	Modeling hydroxylated nanosilica: Testing the performance of ReaxFF and FFSiOH force fields. Journal of Chemical Physics, 2017, 146, 224704.	1.2	12
122	Self-diffusion of molecular hydrogen in clathrasils compared: Dodecasil 3C versus sodalite. Journal of Chemical Physics, 2005, 122, 204710.	1.2	11
123	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
124	Zeolite synthesis: an energetic perspective. Physical Chemistry Chemical Physics, 2010, 12, 14579.	1.3	11
125	Nanoscale thermal stabilization via permutational premelting. Physical Review B, 2012, 85, .	1.1	11
126	Evidence of intrinsic ambipolar charge transport in a high band gap organic semiconductor. Journal of Materials Chemistry, 2012, 22, 345-348.	6.7	11

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127	Assessing the viability of silicate nanoclusters as carriers of the anomalous microwave emission: a quantum mechanical study. Astronomy and Astrophysics, 2020, 634, A77.	2.1	11
128	Neutral Organic Radical Formation by Chemisorption on Metal Surfaces. Journal of Physical Chemistry Letters, 2020, 11, 3897-3904.	2.1	11
129	Xâ€ray Detectors With Ultrahigh Sensitivity Employing High Performance Transistors Based on a Fully Organic Small Molecule Semiconductor/Polymer Blend Active Layer. Advanced Electronic Materials, 2022, 8, .	2.6	11
130	A computational study into the viability of new molecular materials polymorphs based on fully-coordinated inorganic nanoclusters. CrystEngComm, 2007, 9, 463.	1.3	10
131	Structural and electronic characterisation of Ï€-extended tetrathiafulvalene derivatives as active components in field-effect transistors. CrystEngComm, 2016, 18, 6149-6152.	1.3	10
132	Direct covalent grafting of an organic radical core on gold and silver. RSC Advances, 2017, 7, 20076-20083.	1.7	10
133	Properties of hydrated TiO₂ and SiO₂ nanoclusters: dependence on size, temperature and water vapour pressure. Nanoscale, 2018, 10, 21518-21532.	2.8	10
134	Computational Modeling of Active Sites in Heterogeneous Catalysts. Cattech, 2003, 7, 164-175.	2.6	9
135	Structure and energetics of hydroxylated silica clusters, (SiO2)M(H2O)N, M=8, 16 and N=1â^'4: A global optimisation study. Chemical Physics Letters, 2012, 554, 117-122.	1.2	9
136	Magic Numbers in a One-Dimensional Nanosystem: ZnS Single-Walled Nanotubes. Journal of Physical Chemistry C, 2013, 117, 22908-22914.	1.5	9
137	From monomer to monolayer: a global optimisation study of (ZnO)_n nanoclusters on the Ag surface. Nanoscale, 2014, 6, 14754-14765.	2.8	9
138	Evidence for multi-polymorphic islands during epitaxial growth of ZnO on Ag(1â€‰1â€‰1). Journal of Physics Condensed Matter, 2016, 28, 224007.	0.7	9
139	Efficient preparation of TiO2 nanoparticle models using interatomic potentials. Journal of Chemical Physics, 2019, 150, 214305.	1.2	9
140	Twistable dipolar aryl rings as electric field actuated conformational molecular switches. Physical Chemistry Chemical Physics, 2021, 23, 3844-3855.	1.3	9
141	How Does Temperature Affect the Infrared Vibrational Spectra of Nanosized Silicate Dust?. ACS Earth and Space Chemistry, 2021, 5, 812-823.	1.2	9
142	Understanding H₂ Formation on Hydroxylated Pyroxene Nanoclusters: Ab Initio Study of the Reaction Energetics and Kinetics. Journal of Physical Chemistry A, 2019, 123, 9282-9291.	1.1	8
143	Magnetism and energetics of the 4d bimetallic cluster Pd6Ru6. International Journal of Quantum Chemistry, 2003, 91, 270-276.	1.0	7
144	Predicting the low energy landscape of nanoscale silica using interatomic potentials. Physica Status Solidi (A) Applications and Materials Science, 2006, 203, 1319-1323.	0.8	7

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145	Influence of Intermolecular Interactions on the Formation of Tetra(carbomethoxy)â€tetrathiafulvalene Assemblies. ChemPhysChem, 2007, 8, 1565-1571.	1.0	7
146	Structural Correspondences between the Low-Energy Nanoclusters of Silica and Water. Journal of Physical Chemistry C, 2008, 112, 18417-18425.	1.5	7
147	Long range coupling between defect centres in inorganic nanostructures: Valence alternation pairs in nanoscale silica. Journal of Chemical Physics, 2012, 137, 154313.	1.2	7
148	Low-energy nanoscale clusters of (TiC) n nÂ=Â6, 12: a structural and energetic comparison with MgO. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	7
149	Study of the Eâ€“Z stilbene isomerisation in perchlorotriphenyl-methane (PTM) derivatives. RSC Advances, 2017, 7, 15278-15283.	1.7	7
150	From cluster calculations to molecular materials: a mixed pseudopotential approach to modeling mixed-valence systems. Journal of Molecular Modeling, 2005, 11, 288-292.	0.8	6
151	Comparing the influence of framework type on H2 absorption in hypothetical and existing clathrasils: a grand canonical Monte Carlo study. Journal of Materials Chemistry, 2006, 16, 3285.	6.7	6
152	One-dimensional embedded cluster approach to modeling CdS nanowires. Journal of Chemical Physics, 2013, 139, 124101.	1.2	6
153	A theoretical study of a ZnO graphene analogue: adsorption on Ag(111) and hydrogen transport. Journal of Physics Condensed Matter, 2011, 23, 334215.	0.7	5
154	Interplay between Magnetism and Magicness in Nanoclusters. Journal of Physical Chemistry C, 2012, 116, 20625-20632.	1.5	5
155	Triarylmethyl-based 2D covalent networks: virtual screening of chemical functionalisation for optimising strain-induced property control. Physical Chemistry Chemical Physics, 2018, 20, 5028-5035.	1.3	4
156	Introduction to modeling nanoclusters and nanoparticles. Frontiers of Nanoscience, 2018, 12, 1-54.	0.3	4
157	Oxygen Vacancies in Oxide Nanoclusters: When Silica Is More Reducible Than Titania. Frontiers in Chemistry, 2019, 7, 37.	1.8	4
158	Effect of spin ordering on structure and structural transitions in the (MnS)6 magic cluster. Chemical Physics Letters, 2013, 556, 207-210.	1.2	3
159	Computing Free Energies of Hydroxylated Silica Nanoclusters: Forcefield versus Density Functional Calculations. Inorganics, 2017, 5, 41.	1.2	3
160	Does Processing or Formation of Water Ice Mantles Affect the Capacity of Nanosilicates to Be the Source of Anomalous Microwave Emission?. Frontiers in Astronomy and Space Sciences, 2021, 8, .	1.1	3
161	Functionalising the gate dielectric of organic field-effect transistors with self-assembled monolayers: effect of molecular electronic structure on device performance. Applied Physics A: Materials Science and Processing, 2022, 128, 1.	1.1	3
162	Molecular Dynamics-based Approach to Study the Anisotropic Self-Diffusion of Molecules in Porous Materials with Multiple Cage Types:Â Application to H2in Losod. Journal of Physical Chemistry B, 2006, 110, 501-506.	1.2	2

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163	Low-energy nanoscale clusters of (TiC)n n = 6, 12: a structural and energetic comparison with MgO. Highlights in Theoretical Chemistry, 2014, , 213-218.	0.0	2
164	Formation of Interstellar Silicate Dust via Nanocluster Aggregation: Insights From Quantum Chemistry Simulations. Frontiers in Astronomy and Space Sciences, 2021, 8, .	1.1	2
165	Cosmic and Atmospheric Nanosilicates. Series in Materials Science and Engineering, 2016, , 369-412.	0.1	1
166	Silicate Nanoclusters: Understanding Their Cosmic Relevance from Bottom-Up Modelling. Challenges and Advances in Computational Chemistry and Physics, 2017, , 237-268.	0.6	1
167	Can calculated harmonic vibrational spectra rationalize the structure of TiC-based nanoparticles?. Physical Chemistry Chemical Physics, 2022, 24, 778-785.	1.3	1
168	Efficiency of Interstellar Nanodust Heating: Accurate Bottom-up Calculations of Nanosilicate Specific Heat Capacities. Journal of Physical Chemistry A, 2022, 126, 3854-3862.	1.1	1
169	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
170	Toward Understanding the Thermodynamic Viability of Zeolites and Related Frameworks Through a Simple Topological Model.. ChemInform, 2004, 35, no.	0.1	0
171	Silica as an Exceptionally Versatile Nanoscale Building Material. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2010, 1, 383-413.	0.6	0
172	On the onset of dust formation in AGB stars. Proceedings of the International Astronomical Union, 2018, 14, 119-128.	0.0	0
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