

Michelle J S Spencer

List of Publications by Year in descending order

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108
papers

3,206
citations

147801
31
h-index

175258
52
g-index

111
all docs

111
docs citations

111
times ranked

4401
citing authors

#	ARTICLE	IF	CITATIONS
1	Gas sensing applications of 1D-nanostructured zinc oxide: Insights from density functional theory calculations. Progress in Materials Science, 2012, 57, 437-486.	32.8	195
2	Electronic Tuning of 2D MoS ₂ through Surface Functionalization. Advanced Materials, 2015, 27, 6225-6229.	21.0	194
3	Density functional theory study of the relaxation and energy of iron surfaces. Surface Science, 2002, 513, 389-398.	1.9	154
4	Fully Light-Controlled Memory and Neuromorphic Computation in Layered Black Phosphorus. Advanced Materials, 2021, 33, e2004207.	21.0	147
5	Ambient Protection of Few-Layer Black Phosphorus via Sequestration of Reactive Oxygen Species. Advanced Materials, 2017, 29, 1700152.	21.0	141
6	Liquid Metals in Catalysis for Energy Applications. Joule, 2020, 4, 2290-2321.	24.0	106
7	ZnO Nanostructures for Gas Sensing: Interaction of NO ₂ , NO, O, and N with the ZnO(101̄...0) Surface. Journal of Physical Chemistry C, 2010, 114, 10881-10893.	3.1	101
8	Multifunctional Optoelectronics via Harnessing Defects in Layered Black Phosphorus. Advanced Functional Materials, 2019, 29, 1901991.	14.9	97
9	Monolayer-to-bilayer transformation of silicenes and their structural analysis. Nature Communications, 2016, 7, 10657.	12.8	88
10	Activity of ZnO polar surfaces: an insight from surface energies. Physical Chemistry Chemical Physics, 2014, 16, 22139-22144.	2.8	87
11	2D/3D Hybrid of MoS ₂ /GaN for a High-Performance Broadband Photodetector. ACS Applied Electronic Materials, 2021, 3, 2407-2414.	4.3	70
12	Adsorption of NO ₂ on Oxygen Deficient ZnO(21̄...1̄...0) for Gas Sensing Applications: A DFT Study. Journal of Physical Chemistry C, 2010, 114, 16603-16610.	3.1	67
13	Liquid-Metal Synthesized Ultrathin SnS Layers for High-Performance Broadband Photodetectors. Advanced Materials, 2020, 32, e2004247.	21.0	66
14	A New Surface and Structure for Silicene: Polygonal Silicene Formation on the Al(111) Surface. Journal of Physical Chemistry C, 2013, 117, 22142-22148.	3.1	62
15	First-principles study of structural and electronic properties of ultrathin silicon nanosheets. Physical Review B, 2010, 82, .	3.2	52
16	Adsorption of NO and NO ₂ on the ZnO() surface: A DFT study. Surface Science, 2009, 603, 3389-3399.	1.9	49
17	Surface reconstruction of ultrathin silicon nanosheets. Chemical Physics Letters, 2011, 506, 221-225.	2.6	47
18	Electrically Activated UV-A Filters Based on Electrochromic MoO ₃ . ACS Applied Materials & Interfaces, 2020, 12, 16997-17003.	8.0	45

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19	Direct conversion of CO ₂ to solid carbon by Ga-based liquid metals. Energy and Environmental Science, 2022, 15, 595-600.	30.8	45
20	A Simplified Method for the 3D Printing of Molecular Models for Chemical Education. Journal of Chemical Education, 2018, 95, 88-96.	2.3	44
21	Maximum piezoelectricity in a few unit-cell thick planar ZnO – A liquid metal-based synthesis approach. Materials Today, 2021, 44, 69-77.	14.2	44
22	Sulfur adsorption on Fe(110): a DFT study. Surface Science, 2003, 540, 420-430.	1.9	42
23	A DFT study of the perovskite and hexagonal phases of BaTiO ₃ . Computational Materials Science, 2005, 34, 157-165.	3.0	41
24	Chirality-2: Development of a Multilevel Mobile Gaming App To Support the Teaching of Introductory Undergraduate-Level Organic Chemistry. Journal of Chemical Education, 2018, 95, 1216-1220.	2.3	41
25	Effect of ZnO Nanostructure Morphology on the Sensing of H ₂ S Gas. Journal of Physical Chemistry C, 2013, 117, 26106-26118.	3.1	39
26	Interaction of hydrogen with ZnO nanopowders – evidence of hydroxyl group formation. Nanotechnology, 2012, 23, 015705.	2.6	38
27	Electrically Sorted Single-Walled Carbon Nanotubes-Based Electron Transporting Layers for Perovskite Solar Cells. IScience, 2019, 14, 100-112.	4.1	36
28	The electronic and structural properties of novel organomodified Si nanosheets. Physical Chemistry Chemical Physics, 2011, 13, 15418.	2.8	35
29	Density functional theory modelling of and surfaces: Structure, properties and adsorption of N ₂ O. Materials Chemistry and Physics, 2010, 119, 505-514.	4.0	34
30	Reconstruction and electronic properties of silicon nanosheets as a function of thickness. Nanoscale, 2012, 4, 2906.	5.6	34
31	Predicting Thermal Properties of Crystals Using Machine Learning. Advanced Theory and Simulations, 2020, 3, 1900208.	2.8	34
32	Chemical modification of group IV graphene analogs. Science and Technology of Advanced Materials, 2018, 19, 76-100.	6.1	33
33	H ₂ S dissociation on the Fe(100) surface: An ab initio molecular dynamics study. Surface Science, 2008, 602, 1547-1553.	1.9	32
34	Anion secondary batteries utilizing a reversible BF ₄ insertion/extraction two-dimensional Si material. Journal of Materials Chemistry A, 2014, 2, 7588.	10.3	32
35	Micro versus macro solid phase extraction for monitoring water contaminants: A preliminary study using trihalomethanes. Science of the Total Environment, 2015, 512-513, 210-214.	8.0	30
36	Structural-Defect-Mediated Grafting of Alkylamine on Few-Layer MoS ₂ and Its Potential for Enhancement of Tribological Properties. ACS Applied Materials & Interfaces, 2020, 12, 30720-30730.	8.0	30

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37	How silicene on Ag(111) oxidizes: microscopic mechanism of the reaction of O ₂ with silicene. Scientific Reports, 2015, 5, 17570.	3.3	28
38	Ordered-vacancy-enabled indium sulphide printed in wafer-scale with enhanced electron mobility. Materials Horizons, 2020, 7, 827-834.	12.2	27
39	Surface Reactions of Ethylene Carbonate and Propylene Carbonate on the Li(001) Surface. Electrochimica Acta, 2017, 243, 320-330.	5.2	26
40	Coverage-Dependent Adsorption of Atomic Sulfur on Fe(110): A DFT Study. Journal of Physical Chemistry B, 2005, 109, 9604-9612.	2.6	25
41	Ab Initio Molecular Dynamics Study of H ₂ S Dissociation on the Fe(110) Surface. Journal of Physical Chemistry C, 2007, 111, 16372-16378.	3.1	24
42	Assessment of arsenic in Australian grown and imported rice varieties on sale in Australia and potential links with irrigation practises and soil geochemistry. Chemosphere, 2015, 138, 1008-1013.	8.2	24
43	Stability of Boronium Cation-Based Ionic Liquid Electrolytes on the Li Metal Anode Surface. ACS Applied Energy Materials, 2020, 3, 5497-5509.	5.1	24
44	Broad-Spectrum Solvent-free Layered Black Phosphorus as a Rapid Action Antimicrobial. ACS Applied Materials & Interfaces, 2021, 13, 17340-17352.	8.0	24
45	Surface defects on ZnO nanowires: implications for design of sensors. Journal of Physics Condensed Matter, 2012, 24, 305001.	1.8	23
46	Zinc oxide for gas sensing of formaldehyde: Density functional theory modelling of the effect of nanostructure morphology and gas concentration on the chemisorption reaction. Materials Chemistry and Physics, 2017, 193, 274-284.	4.0	23
47	Effect of nanostructuring of ZnO for gas sensing of nitrogen dioxide. Computational Materials Science, 2017, 132, 104-115.	3.0	23
48	Mechanochemical lithiation of layered polysilane. Chemical Communications, 2014, 50, 9761-9764.	4.1	21
49	Effect of S contamination on properties of Fe(100) surfaces. Surface Science, 2005, 590, 63-75.	1.9	20
50	The interaction of ethylammonium tetrafluoroborate [EtNH ₃ ⁺][BF ₄ ⁻] ionic liquid on the Li(001) surface: towards understanding early SEI formation on Li metal. Physical Chemistry Chemical Physics, 2019, 21, 10028-10037.	2.8	20
51	Further studies of iron adhesion: () surfaces. Surface Science, 2002, 515, L464-L468.	1.9	19
52	Ab initio study of S dynamics on iron surfaces. Surface Science, 2007, 601, 665-671.	1.9	19
53	Effect of S Arrangement on Fe(110) Properties at 1/3 Monolayer Coverage: A DFT Study. Journal of Physical Chemistry B, 2006, 110, 956-962.	2.6	18
54	Adsorption of toxic gases on silicene/Ag(111). Physical Chemistry Chemical Physics, 2019, 21, 17521-17537.	2.8	17

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55	Mixed Ionic–Electronic Charge Transport in Layered Black–Phosphorus for Low–Power Memory. <i>Advanced Functional Materials</i> , 2022, 32, 2107068.	14.9	16
56	Generating strong room-temperature photoluminescence in black phosphorus using organic molecules. <i>2D Materials</i> , 2019, 6, 015009.	4.4	15
57	Adsorption of silane and methylsilane on gold surfaces. <i>Surface Science</i> , 2004, 573, 151-168.	1.9	14
58	Monocrystalline Antimonene Nanosheets via Physical Vapor Deposition. <i>Advanced Materials Interfaces</i> , 2020, 7, 2001678.	3.7	14
59	Alkali-Assisted Hydrothermal Exfoliation and Surfactant-Driven Functionalization of <i>h</i> -BN Nanosheets for Lubrication Enhancement. <i>ACS Applied Nano Materials</i> , 2021, 4, 9143-9154.	5.0	14
60	DFT modelling of hydrogen on Cu(110)- and (111)-type clusters. <i>Molecular Simulation</i> , 2002, 28, 807-825.	2.0	13
61	Effect of Sulfur Impurity on Fe(110) Adhesion: A DFT Study. <i>Journal of Physical Chemistry B</i> , 2004, 108, 10965-10972.	2.6	13
62	Adsorption of atomic nitrogen and oxygen on $\text{ZnO}(2\text{ar } \{1\} \text{ ar } \{1\}0\}$ surface: a density functional theory study. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 144208.	1.8	13
63	Interactions between stacked layers of phenyl-modified silicene. <i>New Journal of Physics</i> , 2013, 15, 125018.	2.9	13
64	Development of Stable Boron Nitride Nanotube and Hexagonal Boron Nitride Dispersions for Electrophoretic Deposition. <i>Langmuir</i> , 2020, 36, 3425-3438.	3.5	13
65	Tuning the work function of the silicene/4 Å– 4 Ag(111) surface. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7165-7173.	2.8	11
66	Soft X-ray Detectors Based on SnS Nanosheets for the Water Window Region. <i>Advanced Functional Materials</i> , 2022, 32, 2105038.	14.9	11
67	Tuning the Schottky barrier height in a multiferroic $\text{In}_2\text{Se}_3/\text{Fe}_3\text{GeTe}_2$ van der Waals heterojunction. <i>Nanoscale</i> , 2021, , .	5.6	11
68	Surface Functionalization of WS_2 Nanosheets with Alkyl Chains for Enhancement of Dispersion Stability and Tribological Properties. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 1334-1346.	8.0	10
69	Adsorption of methylsilane on copper surfaces. <i>Surface Science</i> , 2003, 543, 162-184.	1.9	9
70	Iron Surfaces: Pathways to Interfaces. <i>Surface Review and Letters</i> , 2003, 10, 169-174.	1.1	9
71	Adsorption of NO_2 on YSZ(111) and Oxygen-Enriched YSZ(111) Surfaces. <i>Journal of Physical Chemistry C</i> , 2013, 117, 12472-12482.	3.1	9
72	Differential Work-Function Enabled Bifunctional Switching in Strontium Titanate Flexible Resistive Memories. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 7326-7333.	8.0	9

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73	Nicotine Sensors for Wearable Battery-Free Monitoring of Vaping. ACS Sensors, 2022, 7, 82-88.	7.8	9
74	Infrared Spectroscopy-Based Metabolomic Analysis for the Detection of Preharvest Sprouting in Grain. Cereal Chemistry, 2016, 93, 444-449.	2.2	8
75	Phenol-Modified Silicene: Preferred Substitution Site and Electronic Properties. Journal of Physical Chemistry C, 2016, 120, 6762-6770.	3.1	8
76	Using 3D Printing to Visualize 2D Chromatograms and NMR Spectra for the Classroom. Journal of Chemical Education, 2021, 98, 1024-1030.	2.3	8
77	Adsorption of SiH ₄ on copper () and () surfaces. Surface Science, 2002, 505, 308-324.	1.9	7
78	Effect of Sulfur Coverage on Fe(110) Adhesion: A DFT Study. Journal of Physical Chemistry B, 2005, 109, 10204-10212.	2.6	7
79	Interaction of hydrogen with zinc oxide nanorods: why the spacing is important. Nanotechnology, 2011, 22, 135704.	2.6	7
80	Catalytic potential of highly defective (211) surfaces of zinc blende ZnO. Physical Chemistry Chemical Physics, 2015, 17, 27683-27689.	2.8	7
81	Manipulation of carbon nanotube magnetism with metal-rich iron nanoparticles. Journal of Materials Chemistry C, 2016, 4, 1215-1227.	5.5	7
82	Spectroscopic and Computational Study of Boronium Ionic Liquids and Electrolytes. Chemistry - A European Journal, 2021, 27, 12826-12834.	3.3	7
83	Tuning the band gap of silicene by functionalisation with naphthyl and anthracyl groups. Journal of Chemical Physics, 2016, 144, 114704.	3.0	6
84	Uncovering New Buckled Structures of Bilayer GaN: A First-Principles Study. Journal of Physical Chemistry C, 2019, 123, 1939-1947.	3.1	6
85	Combining computational and experimental approaches to select chromophores to enable the detection of fatty acids via HPLC. Analytical Methods, 2019, 11, 2952-2959.	2.7	5
86	Interplay of Mechanical and Chemical Tunability of Phosphorene for Flexible Nanoelectronic Applications. Journal of Physical Chemistry C, 2020, 124, 24391-24399.	3.1	5
87	The (In)Stability of the Ionic Liquids [(TMEDA)BH ₂][TFSI] and [FSI] on the Li(001) Surface. Batteries and Supercaps, 2021, 4, 1126-1134.	4.7	5
88	Improving sensing of formaldehyde using ZnO nanostructures with surface-adsorbed oxygen. Nanoscale Advances, 2022, 4, 546-561.	4.6	5
89	Hydrogen bonding in mixed ligand copper organophosphonates. Chemical Physics Letters, 2003, 378, 400-405.	2.6	4
90	Density Functional Theory and ab Initio Molecular Dynamics Investigation of Hydronium Interactions with Graphene. Energy Procedia, 2017, 110, 518-522.	1.8	4

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91	Fluorinated Boron-Based Anions for Higher Voltage Li Metal Battery Electrolytes. <i>Nanomaterials</i> , 2021, 11, 2391.	4.1	4
92	Electrochemical Stability of Zinc and Copper Surfaces in Protic Ionic Liquids. <i>Langmuir</i> , 2022, 38, 4633-4644.	3.5	4
93	Towards higher electrochemical stability of electrolytes: lithium salt design through <i>in silico</i> screening. <i>Journal of Materials Chemistry A</i> , 2022, 10, 13254-13265.	10.3	4
94	The adsorption of NO on YSZ(111) and oxygen-enriched YSZ(111) surfaces. <i>Chemical Physics Letters</i> , 2014, 593, 61-68.	2.6	3
95	The interaction of several fluorinated ionic liquids on the LiF(001) surface. <i>Surfaces and Interfaces</i> , 2021, 22, 100836.	3.0	3
96	Black Phosphorus-Diketopyrrolopyrrole Polymer Semiconductor Hybrid for Enhanced Charge Transfer and Photodetection. <i>Advanced Photonics Research</i> , 2021, 2, 2100150.	3.6	3
97	Mono- to few-layer non-van der Waals 2D lanthanide-doped NaYF ₄ nanosheets with upconversion luminescence. <i>2D Materials</i> , 2021, 8, 015005.	4.4	3
98	Reactive Oxygen Species Sequestration Induced Synthesis of β -PbO and Its Polymorphic Transformation to γ -PbO at Atomically Thin Regimes. <i>ACS Nano</i> , 2022, 16, 10679-10691.	14.6	3
99	Density functional theory calculations of phenol-modified monolayer silicon nanosheets. , 2013, , .		2
100	Theoretical insight on the origin of anelasticity in zinc oxide nanowires. <i>Nanoscale</i> , 2020, 12, 2439-2444.	5.6	2
101	Broadband Photodetectors: Liquid-Metal Synthesized Ultrathin SnS Layers for High-Performance Broadband Photodetectors (<i>Adv. Mater.</i> 45/2020). <i>Advanced Materials</i> , 2020, 32, 2070338.	21.0	2
102	Theoretical Studies of Functionalised Silicene. <i>Springer Series in Materials Science</i> , 2016, , 107-127.	0.6	1
103	Role of Surface Paramagnetic Oxygen Species in the Desulfurization Reactions on Zinc Oxide. <i>Journal of Physical Chemistry C</i> , 2021, 125, 4559-4566.	3.1	1
104	Guest Editorial Introduction. <i>Molecular Simulation</i> , 2016, 42, 447-447.	2.0	0
105	The science and life of Ian K. Snook. <i>Molecular Simulation</i> , 2016, 42, 448-457.	2.0	0
106	Elemental Two-Dimensional Materials Beyond Graphene. <i>ChemistrySelect</i> , 2017, 2, .	1.5	0
107	Zero valence iron nanocube decoration of graphitic nanoplatelets. <i>Nanotechnology</i> , 2022, 33, 025704.	2.6	0
108	Understanding the Link between Anion Structure and Lithium Coordination. <i>ECS Meeting Abstracts</i> , 2019, , .	0.0	0