Dean C Sayle

List of Publications by Year
in descending order

112 papers	5,573 citations	126708 33 h-index	79541 73 g-index
119 all docs	119 docs citations	119 times ranked	6886 citing authors

#	Article	IF	Citations
1	Reduced Graphene Oxide Conjugated Cu₂O Nanowire Mesocrystals for High-Performance NO₂ Gas Sensor. Journal of the American Chemical Society, 2012, 134, 4905-4917.	6.6	706
2	Density functional theory studies of the structure and electronic structure of pure and defective low index surfaces of ceria. Surface Science, 2005, 576, 217-229.	0.8	683
3	Converting Ceria Polyhedral Nanoparticles into Single-Crystal Nanospheres. Science, 2006, 312, 1504-1508.	6.0	570
4	Atomistic Models for CeO2(111), (110), and (100) Nanoparticles, Supported on Yttrium-Stabilized Zirconia. Journal of the American Chemical Society, 2002, 124, 11429-11439.	6.6	248
5	The induction of angiogenesis by cerium oxide nanoparticles through the modulation of oxygen in intracellular environments. Biomaterials, 2012, 33, 7746-7755.	5.7	247
6	Exploring the properties and applications of nanoceria: is there still plenty of room at the bottom?. Environmental Science: Nano, 2014, 1, 390-405.	2.2	218
7	Water Adsorption and Its Effect on the Stability of Low Index Stoichiometric and Reduced Surfaces of Ceria. Journal of Physical Chemistry C, 2012, 116, 7073-7082.	1.5	204
8	Cellular Interaction and Toxicity Depend on Physicochemical Properties and Surface Modification of Redox-Active Nanomaterials. ACS Nano, 2013, 7, 4855-4868.	7.3	179
9	Oxidising CO to CO2 using ceria nanoparticles. Physical Chemistry Chemical Physics, 2005, 7, 2936.	1.3	159
10	Strain and Architecture-Tuned Reactivity in Ceria Nanostructures; Enhanced Catalytic Oxidation of CO to CO₂. Chemistry of Materials, 2012, 24, 1811-1821.	3.2	100
11	Behavior of nanoceria in biologically-relevant environments. Environmental Science: Nano, 2014, 1, 516-532.	2.2	94
12	Shape of CeO2 nanoparticles using simulated amorphisation and recrystallisation. Chemical Communications, 2004, , 2438.	2.2	84
13	Engineered defects in cerium oxides: tuning chemical reactivity for biomedical, environmental, & energy applications. Nanoscale, 2020, 12, 6879-6899.	2.8	79
14	Predicting the Electrochemical Properties of MnO₂ Nanomaterials Used in Rechargeable Li Batteries: Simulating Nanostructure at the Atomistic Level. Journal of the American Chemical Society, 2009, 131, 6161-6173.	6.6	74
15	Environment-mediated structure, surface redox activity and reactivity of ceria nanoparticles. Nanoscale, 2013, 5, 6063.	2.8	71
16	Generating MnO2Nanoparticles Using Simulated Amorphization and Recrystallization. Journal of the American Chemical Society, 2005, 127, 12828-12837.	6.6	69
17	Computer simulation of thin film heteroepitaxial ceramic interfaces using a near-coincidence-site lattice theory. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1993, 68, 565-573.	0.8	61
18	â€œSimulating Synthesisâ€Â Ceria Nanosphere Self-Assembly into Nanorods and Framework Architectures. Journal of the American Chemical Society, 2007, 129, 7924-7935.	6.6	58

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19	Computer simulation study of the defect chemistry of rutile TiO2. Journal of Physics and Chemistry of Solids, 1995, 56, 799-805.	1.9	54
20	Cationic Surface Reconstructions on Cerium Oxide Nanocrystals: An Aberration-Corrected HRTEM Study. ACS Nano, 2012, 6, 421-430.	7.3	53
21	Structureâ€“Activity Map of Ceria Nanoparticles, Nanocubes, and Mesoporous Architectures. Chemistry of Materials, 2016, 28, 7287-7295.	3.2	53
22	Is Geometric Frustration-Induced Disorder a Recipe for High Ionic Conductivity?. Journal of the American Chemical Society, 2017, 139, 5842-5848.	6.6	53
23	Engineering of nanoscale defect patterns in CeO₂ nanorods via ex situ and in situ annealing. Nanoscale, 2015, 7, 5169-5177.	2.8	51
24	Mapping Nanostructure: A Systematic Enumeration of Nanomaterials by Assembling Nanobuilding Blocks at Crystallographic Positions. ACS Nano, 2008, 2, 1237-1251.	7.3	50
25	Computer Modeling of the Active-Site Configurations within the NO Decomposition Catalyst Cu-ZSM-5. Journal of Physical Chemistry A, 1997, 101, 3331-3337.	1.1	46
26	Computer Modeling of the V2O5/TiO2Interface. The Journal of Physical Chemistry, 1996, 100, 8940-8945.	2.9	45
27	Ionic conductivity in nano-scale CeO2/YSZ heterolayers. Journal of Materials Chemistry, 2006, 16, 1067.	6.7	45
28	Morphological Phase Diagram of Biocatalytically Active Ceria Nanostructures as a Function of Processing Variables and Their Properties. ChemPlusChem, 2013, 78, 1446-1455.	1.3	45
29	Mechanical properties of ceria nanorods and nanochains; the effect of dislocations, grain-boundaries and oriented attachment. Nanoscale, 2011, 3, 1823.	2.8	42
30	Dynamics of Polar Surfaces on Ceria Nanoparticles Observed In Situ with Singleâ€Atom Resolution. Advanced Functional Materials, 2011, 21, 1971-1976.	7.8	40
31	Ethylbenzene dehydrogenation on Fe2O3-Cr2O3-K2CO3 catalysts promoted with transitional metal oxides. Applied Catalysis A: General, 2005, 287, 9-18.	2.2	38
32	Morphology and Crystal Planes Effects on Supercapacitance of CeO₂ Nanostructures: Electrochemical and Molecular Dynamics Studies. Particle and Particle Systems Characterization, 2018, 35, 1800176.	1.2	38
33	Selfâ€Assembly of Cerium Oxide Nanostructures in Ice Molds. Small, 2008, 4, 1210-1216.	5.2	37
34	Atomistic Modeling of Multilayered Ceria Nanotubes. Nano Letters, 2007, 7, 543-546.	4.5	33
35	Morphology and Surface Analysis of Pure and Doped Cuboidal Ceria Nanoparticles. Journal of Physical Chemistry C, 2013, 117, 24561-24569.	1.5	31
36	The stability of defects in the ceramic interfaces, and. Surface Science, 1995, 334, 170-178.	0.8	30

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37	Computer Simulation of Surface Segregation. Molecular Simulation, 1992, 9, 83-98.	0.9	27
38	Computer modelling of V2O5: surface structures, crystal morphology and ethene sorption. Journal of Materials Chemistry, 1996, 6, 653.	6.7	26
39	Strongly Bound Surface Water Affects the Shape Evolution of Cerium Oxide Nanoparticles. Journal of Physical Chemistry C, 2020, 124, 3577-3588.	1.5	26
40	Computer-Aided Design of Nanoceria Structures as Enzyme Mimetic Agents: The Role of Bodily Electrolytes on Maximizing Their Activity. ACS Applied Bio Materials, 2019, 2, 1098-1106.	2.3	25
41	Controlling the {111}/{110} Surface Ratio of Cuboidal Ceria Nanoparticles. ACS Applied Materials & Interfaces, 2019, 11, 11384-11390.	4.0	25
42	The predicted 3-D atomistic structure of an interfacial screwâ€“edge dislocation. Journal of Materials Chemistry, 1999, 9, 2961-2964.	6.7	24
43	Atomistic simulation methodologies for modelling the nucleation, growth and structure of interfaces. Journal of Materials Chemistry, 2000, 10, 1315-1324.	6.7	24
44	Atomistic structure of oxide nanoparticles supported on an oxide substrate. Physical Review B, 2002, 65, .	1.1	24
45	Oxygen transport in unreduced, reduced and Rh(iii)-doped CeO2nanocrystals. Faraday Discussions, 2007, 134, 377-397.	1.6	24
46	Modelling oxide thin films. Molecular Simulation, 2002, 28, 683-725.	0.9	23
47	Simulating Mechanical Deformation in Nanomaterials with Application for Energy Storage in Nanoporous Architectures. ACS Nano, 2009, 3, 3308-3314.	7.3	23
48	Evolutionary techniques in atomistic simulation: thin films and nanoparticles. Current Opinion in Solid State and Materials Science, 2003, 7, 3-12.	5.6	22
49	Computer aided design of nano-structured materials with tailored ionic conductivities. Physical Chemistry Chemical Physics, 2005, 7, 16.	1.3	22
50	Simulating Self-Assembly of ZnS Nanoparticles into Mesoporous Materials. Journal of the American Chemical Society, 2006, 128, 15283-15291.	6.6	22
51	Elastic Deformation in Ceria Nanorods via a Fluorite-to-Rutile Phase Transition. ACS Nano, 2010, 4, 879-886.	7.3	22
52	Amorphization and recrystallization study of lithium insertion into manganese dioxide. Physical Chemistry Chemical Physics, 2011, 13, 1307-1313.	1.3	20
53	Origin of electrochemical activity in nano-Li₂MnO₃; stabilization via a â€˜point defect scaffoldâ€™. Nanoscale, 2015, 7, 1167-1180.	2.8	20
54	Effect of defects on the stability of heteroepitaxial ceramic interfaces studied by computer simulation. Physical Review B, 1994, 50, 14498-14505.	1.1	19

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55	Structural exploration of thin-film oxide interfaces via â€˜simulated amorphisation and recrystallisationâ€™. Surface Science, 2001, 473, 97-107.	0.8	19
56	Application of molecular dynamics DL_POLY codes to interfaces of inorganic materials. Molecular Simulation, 2006, 32, 1079-1093.	0.9	19
57	Simulated amorphisation and recrystallisation: nanocrystallites within meso-scale supported oxides. Journal of Materials Chemistry, 2000, 10, 2241-2243.	6.7	18
58	Dislocations, lattice slip, defects and rotated domains: The effect of a lattice misfit on supported thin-film metal oxides. Physical Chemistry Chemical Physics, 2000, 2, 5491-5499.	1.3	18
59	Active site configurations within the NO decomposition catalyst, Cu-ZSM-5; the role of framework aluminium. Journal of Materials Chemistry, 1997, 7, 1635-1639.	6.7	16
60	Symmetry-Driven Spontaneous Self-Assembly of Nanoscale Ceria Building Blocks to Fractal Superoctahedra. Crystal Growth and Design, 2009, 9, 1614-1620.	1.4	16
61	Exercising control over the influence of the lattice misfit on the structure of oxideâ€“oxide thin film interfaces. Journal of Materials Chemistry, 1999, 9, 2779-2787.	6.7	15
62	The Atomistic Structures of MgO/SrTiO3(001) and BaO/SrTiO3(001) Using Simulated Amorphization and Recrystallization. Journal of Physical Chemistry B, 2001, 105, 5506-5514.	1.2	15
63	Synthesis, structure and ionic conductivity in nanopolycrystalline BaF2/CaF2 heterolayersElectronic supplementary information (ESI) available: potential parameters and pertinent calculated physical properties for the perfect BaF2 and CaF2. See http://www.rsc.org/suppdata/cc/b3/b305393h/. Chemical Communications, 2003, , 1804.	2.2	15
64	Encapsulated Oxide Nanoparticles:Â The Influence of the Microstructure on Associated Impurities within a Material. Journal of the American Chemical Society, 2003, 125, 8581-8588.	6.6	14
65	Modelling of structure, sorption, synthesis and reactivity in catalytic systems1Communication presented at the First Francqui Colloquium, Brussels, 19â€“20 February 1996.1. Journal of Molecular Catalysis A, 1997, 115, 431-448.	4.8	13
66	Evolving microstructure in MnO2 using amorphisation and recrystallisation. Journal of Crystal Growth, 2006, 294, 118-129.	0.7	13
67	Accommodation of the misfit strain energy in the BaO(100)/MgO(100) heteroepitaxial ceramic interface using computer simulation techniques. Journal of Materials Chemistry, 1994, 4, 1883.	6.7	12
68	Copper clusters in mordenite. A direct structural comparison with the NO decomposition catalyst Cu-ZSM-5. Journal of Materials Chemistry, 1997, 7, 1917-1923.	6.7	12
69	Atomistic Simulation and Characterization of Spinel Li_{1+x}Mn₂O₄ (0 â‰ x â‰ 1) Nanoparticles. ACS Applied Energy Materials, 2020, 3, 1429-1438.	2.5	12
70	High-Pressure Crystallisation of TiO₂ Nanoparticles. Journal of Computational and Theoretical Nanoscience, 2007, 4, 299-308.	0.4	12
71	Simulation study of copper(I) and copper(II) species in ZSM-5 zeolite. Journal of the Chemical Society Chemical Communications, 1995, , 945.	2.0	11
72	A refined model for the active site within the NO decomposition catalyst, Cu-ZSM-5. Microporous and Mesoporous Materials, 1998, 20, 259-267.	2.2	11

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73	Atomistic Structures of 25â€‰000-Atom Oxide Nanoparticles Supported on an Oxide Substrate. Journal of Physical Chemistry B, 2002, 106, 10793-10807.	1.2	11
74	Visualizing The Enhanced Chemical Reactivity of Mesoporous Ceria; Simulating Templated Crystallization in Silica Scaffolds at the Atomic Level. Journal of the American Chemical Society, 2014, 136, 4056-4065.	6.6	11
75	Structural Characterization of the CeO2/YSZ(111) Catalytic System Synthesized Using Simulated Amorphization and Recrystallization. Journal of Physical Chemistry B, 2001, 105, 12481-12489.	1.2	10
76	Inducing Polycrystallinity within Supported Oxide Thin Films Using Template Buffer Layers. Journal of Physical Chemistry B, 2002, 106, 3778-3787.	1.2	10
77	Sorption of ethene and ethane on the V2O5(001)/TiO2(001) anatase interface. Catalysis Letters, 1996, 38, 203-208.	1.4	9
78	Evolution and atomistic structure of dislocations defects and clusters within CeO2 supported on ZrO2. Chemical Communications, 2001, , 289-290.	2.2	9
79	Tuning the Properties of Nanoceria by Applying Force: Stress-Induced Ostwald Ripening. Journal of Physical Chemistry C, 2016, 120, 14337-14344.	1.5	9
80	A Study of Thin Film YBa₂Cu₃O_{6.5}/MgO Interfaces Using a Near Coincidence Site Lattice Theory with Atomistic Simulation. Molecular Simulation, 1994, 12, 127-139.	0.9	8
81	Generating structural distributions of atomistic models of Li2O nanoparticles using simulated crystallisation. Journal of Materials Chemistry, 2010, 20, 10452.	6.7	8
82	Formation and Elimination of Anti-site Defects during Crystallization in Perovskite Ba_{1â€“x}Sr_xLiF₃. Crystal Growth and Design, 2018, 18, 2093-2099.	1.4	8
83	Calculated defect formation energies as a function of distance from the BaO/MgO interface compared with image theory predictions. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1994, 69, 787-792.	0.8	7
84	Simulating the structures of crystals and their surfaces. Topics in Catalysis, 1996, 3, 135-167.	1.3	7
85	The Atomistic Structure of an MgO Cluster, Supported on BaO, Synthesized Using Simulated Amorphization and Recrystallization. Journal of Physical Chemistry B, 2002, 106, 3916-3925.	1.2	7
86	Tomographic Study of Mesopore Formation in Ceria Nanorods. Journal of Physical Chemistry C, 2021, 125, 10077-10089.	1.5	7
87	Strain reduction in supported materials; the formation of cracks and dislocations. Journal of Materials Chemistry, 1999, 9, 607-616.	6.7	6
88	Structure of Surface Entrance Sites for Li Intercalation into TiO₂ Nanoparticles, Nanosheets, and Mesoporous Architectures with Application for Li-Ion Batteries. Journal of Physical Chemistry C, 2016, 120, 14001-14008.	1.5	6
89	Protecting Ceria Nanocatalystsâ€”The Role of Sacrificial Barriers. ACS Applied Materials & Interfaces, 2018, 10, 32510-32515.	4.0	6
90	In-situ observation of radiation physics and chemistry of nanostructured cerium oxide in water. Materials Research Express, 2019, 6, 015032.	0.8	6

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91	Structure, epitaxial growth and nucleation of CaO/SrO interfaces using energy minimisation, molecular dynamics and computer graphics. Journal of Materials Chemistry, 1998, 8, 2025-2032.	6.7	5
92	Metal oxide encapsulated nanoparticles. Journal of Materials Chemistry, 2003, 13, 2078.	6.7	5
93	Nanopolycrystalline materials; a general atomistic model for simulation. Physical Chemistry Chemical Physics, 2010, 12, 8584.	1.3	5
94	X-Ray Absorption Spectroscopy and Computer Modelling Study of Nanocrystalline Binary Alkaline Earth Fluorides. IOP Conference Series: Materials Science and Engineering, 2015, 80, 012005.	0.3	5
95	â€˜Breathing-crystalsâ€™ the origin of electrochemical activity of mesoporous Liâ€“MnO₂. Journal of Materials Chemistry A, 2016, 4, 6456-6464.	5.2	5
96	NaCl clusters on MgO(001):â€ƒA model system to explore interfacial crystal growth, nucleation, and grain-boundary formation. Physical Review B, 1997, 56, 15952-15961.	1.1	4
97	Atomic motion on various surfaces of ceria nanoparticles in comparison. Journal of Physics: Conference Series, 2012, 371, 012007.	0.3	4
98	Liquid crystal seed nucleates liquidâ€“solid phase change in ceria nanoparticles. Physical Chemistry Chemical Physics, 2015, 17, 4441-4447.	1.3	4
99	An Introduction to Molecular Heterogeneous Catalysis. , 1998, , 189-214.		4
100	EXAFS and Raman scattering studies of Y and Zr doped nano-crystalline tin oxide. Journal of Physics: Conference Series, 2010, 249, 012054.	0.3	3
101	Mechanical properties of mesoporous ceria nanoarchitectures. Physical Chemistry Chemical Physics, 2014, 16, 24899-24912.	1.3	3
102	Tuning Antisite Defect Density in Perovskite-BaLiF₃ via Cycling between Ball Milling and Heating. Journal of Physical Chemistry Letters, 2018, 9, 5121-5124.	2.1	3
103	Molecular Simulation of Mineral Surfaces and the Role of Impurities on Surface Stability. AIP Conference Proceedings, 2007, , .	0.3	2
104	Computer Simulation of Structural, Defect and Surface Properties of Solids. , 1997, , 479-521.		2
105	Support Effect in V2o5 / Tio2 Partial Oxidation Catalysts. Oil & Gas Science & Technology, 1996, 51, 43-47.	0.2	2
106	Synthesis of a BaO thin film supported on MgO(001) using a shell-model amorphisation and recrystallisation strategy. Physical Chemistry Chemical Physics, 2002, 4, 5189-5198.	1.3	1
107	SINGLE-ATOM MOVEMENT: Dynamics of Polar Surfaces on Ceria Nanoparticles Observed In Situ with Single-Atom Resolution (Adv. Funct. Mater. 11/2011). Advanced Functional Materials, 2011, 21, 1970-1970.	7.8	1
108	ATOMISTIC MODELLING OF CERIA NANOSTRUCTURES: INTRODUCING STRUCTURAL COMPLEXITY. Catalytic Science Series, 2013, , 247-293.	0.6	1

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109	The influence of a material microstructure on the behaviour of dopants. Journal of Materials Chemistry, 2004, 14, 2380.	6.7	0
110	Atomistic Models and Molecular Dynamics. , 2006, , 247-286.		0
111	Amorphisation and recrystallisation study of lithium intercalation into TiO2 nano-architecture.. IOP Conference Series: Materials Science and Engineering, 2017, 169, 012020.	0.3	0
112	From nanoparticles to mesoporous materials. Frontiers of Nanoscience, 2018, , 129-144.	0.3	0