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	Tomographic Study of Mesopore Formation in Ceria Nanorods. Journal of Physical Chemistry C, 2021, 125, 10077-10089.	1.5	7
2	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
3	Engineered defects in cerium oxides: tuning chemical reactivity for biomedical, environmental, & energy applications. Nanoscale, 2020, 12, 6879-6899.	2.8	79
4	Strongly Bound Surface Water Affects the Shape Evolution of Cerium Oxide Nanoparticles. Journal of Physical Chemistry C, 2020, 124, 3577-3588.	1.5	26
5	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
6	Controlling the {111}/{110} Surface Ratio of Cuboidal Ceria Nanoparticles. ACS Applied Materials & Interfaces, 2019, 11, 11384-11390.	4.0	25
7	In-situ observation of radiation physics and chemistry of nanostructured cerium oxide in water. Materials Research Express, 2019, 6, 015032.	0.8	6
8	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
9	From nanoparticles to mesoporous materials. Frontiers of Nanoscience, 2018, , 129-144.	0.3	0
10	Protecting Ceria Nanocatalystsâ€”The Role of Sacrificial Barriers. ACS Applied Materials & Interfaces, 2018, 10, 32510-32515.	4.0	6
11	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
12	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
13	Amorphisation and recrystallisation study of lithium intercalation into TiO2 nano-architecture.. IOP Conference Series: Materials Science and Engineering, 2017, 169, 012020.	0.3	0
14	Is Geometric Frustration-Induced Disorder a Recipe for High Ionic Conductivity?. Journal of the American Chemical Society, 2017, 139, 5842-5848.	6.6	53
15	â€˜Breathing-crystalsâ€™ the origin of electrochemical activity of mesoporous Liâ€“MnO₂. Journal of Materials Chemistry A, 2016, 4, 6456-6464.	5.2	5
16	Structureâ€“Activity Map of Ceria Nanoparticles, Nanocubes, and Mesoporous Architectures. Chemistry of Materials, 2016, 28, 7287-7295.	3.2	53
17	Tuning the Properties of Nanoceria by Applying Force: Stress-Induced Ostwald Ripening. Journal of Physical Chemistry C, 2016, 120, 14337-14344.	1.5	9
18	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

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19	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
20	Liquid crystal seed nucleates liquidâ€“solid phase change in ceria nanoparticles. Physical Chemistry Chemical Physics, 2015, 17, 4441-4447.	1.3	4
21	Engineering of nanoscale defect patterns in CeO₂ nanorods via ex situ and in situ annealing. Nanoscale, 2015, 7, 5169-5177.	2.8	51
22	Origin of electrochemical activity in nano-Li₂MnO₃; stabilization via a â€˜point defect scaffoldâ€™. Nanoscale, 2015, 7, 1167-1180.	2.8	20
23	Mechanical properties of mesoporous ceria nanoarchitectures. Physical Chemistry Chemical Physics, 2014, 16, 24899-24912.	1.3	3
24	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
25	Behavior of nanoceria in biologically-relevant environments. Environmental Science: Nano, 2014, 1, 516-532.	2.2	94
26	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
27	Cellular Interaction and Toxicity Depend on Physicochemical Properties and Surface Modification of Redox-Active Nanomaterials. ACS Nano, 2013, 7, 4855-4868.	7.3	179
28	Environment-mediated structure, surface redox activity and reactivity of ceria nanoparticles. Nanoscale, 2013, 5, 6063.	2.8	71
29	ATOMISTIC MODELLING OF CERIA NANOSTRUCTURES: INTRODUCING STRUCTURAL COMPLEXITY. Catalytic Science Series, 2013, , 247-293.	0.6	1
30	Morphology and Surface Analysis of Pure and Doped Cuboidal Ceria Nanoparticles. Journal of Physical Chemistry C, 2013, 117, 24561-24569.	1.5	31
31	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
32	Atomic motion on various surfaces of ceria nanoparticles in comparison. Journal of Physics: Conference Series, 2012, 371, 012007.	0.3	4
33	Cationic Surface Reconstructions on Cerium Oxide Nanocrystals: An Aberration-Corrected HRTEM Study. ACS Nano, 2012, 6, 421-430.	7.3	53
34	The induction of angiogenesis by cerium oxide nanoparticles through the modulation of oxygen in intracellular environments. Biomaterials, 2012, 33, 7746-7755.	5.7	247
35	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
36	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

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37	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
38	Mechanical properties of ceria nanorods and nanochains; the effect of dislocations, grain-boundaries and oriented attachment. Nanoscale, 2011, 3, 1823.	2.8	42
39	Amorphization and recrystallization study of lithium insertion into manganese dioxide. Physical Chemistry Chemical Physics, 2011, 13, 1307-1313.	1.3	20
40	Dynamics of Polar Surfaces on Ceria Nanoparticles Observed In Situ with Singleâ€Atom Resolution. Advanced Functional Materials, 2011, 21, 1971-1976.	7.8	40
41	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
42	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
43	Generating structural distributions of atomistic models of Li2O nanoparticles using simulated crystallisation. Journal of Materials Chemistry, 2010, 20, 10452.	6.7	8
44	Elastic Deformation in Ceria Nanorods via a Fluorite-to-Rutile Phase Transition. ACS Nano, 2010, 4, 879-886.	7.3	22
45	Nanopolycrystalline materials; a general atomistic model for simulation. Physical Chemistry Chemical Physics, 2010, 12, 8584.	1.3	5
46	Simulating Mechanical Deformation in Nanomaterials with Application for Energy Storage in Nanoporous Architectures. ACS Nano, 2009, 3, 3308-3314.	7.3	23
47	Symmetry-Driven Spontaneous Self-Assembly of Nanoscale Ceria Building Blocks to Fractal Superoctahedra. Crystal Growth and Design, 2009, 9, 1614-1620.	1.4	16
48	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
49	Selfâ€Assembly of Cerium Oxide Nanostructures in Ice Molds. Small, 2008, 4, 1210-1216.	5.2	37
50	Mapping Nanostructure: A Systematic Enumeration of Nanomaterials by Assembling Nanobuilding Blocks at Crystallographic Positions. ACS Nano, 2008, 2, 1237-1251.	7.3	50
51	Molecular Simulation of Mineral Surfaces and the Role of Impurities on Surface Stability. AIP Conference Proceedings, 2007, , .	0.3	2
52	Oxygen transport in unreduced, reduced and Rh(iii)-doped CeO2nanocrystals. Faraday Discussions, 2007, 134, 377-397.	1.6	24
53	Atomistic Modeling of Multilayered Ceria Nanotubes. Nano Letters, 2007, 7, 543-546.	4.5	33
54	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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55	High-Pressure Crystallisation of TiO₂ Nanoparticles. Journal of Computational and Theoretical Nanoscience, 2007, 4, 299-308.	0.4	12
56	Simulating Self-Assembly of ZnS Nanoparticles into Mesoporous Materials. Journal of the American Chemical Society, 2006, 128, 15283-15291.	6.6	22
57	Application of molecular dynamics DL_POLY codes to interfaces of inorganic materials. Molecular Simulation, 2006, 32, 1079-1093.	0.9	19
58	Converting Ceria Polyhedral Nanoparticles into Single-Crystal Nanospheres. Science, 2006, 312, 1504-1508.	6.0	570
59	Ionic conductivity in nano-scale CeO2/YSZ heterolayers. Journal of Materials Chemistry, 2006, 16, 1067.	6.7	45
60	Atomistic Models and Molecular Dynamics. , 2006, , 247-286.		0
61	Evolving microstructure in MnO2 using amorphisation and recrystallisation. Journal of Crystal Growth, 2006, 294, 118-129.	0.7	13
62	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
63	Ethylbenzene dehydrogenation on Fe2O3-Cr2O3-K2CO3 catalysts promoted with transitional metal oxides. Applied Catalysis A: General, 2005, 287, 9-18.	2.2	38
64	Generating MnO2Nanoparticles Using Simulated Amorphization and Recrystallization. Journal of the American Chemical Society, 2005, 127, 12828-12837.	6.6	69
65	Oxidising CO to CO2 using ceria nanoparticles. Physical Chemistry Chemical Physics, 2005, 7, 2936.	1.3	159
66	Computer aided design of nano-structured materials with tailored ionic conductivities. Physical Chemistry Chemical Physics, 2005, 7, 16.	1.3	22
67	The influence of a material microstructure on the behaviour of dopants. Journal of Materials Chemistry, 2004, 14, 2380.	6.7	0
68	Shape of CeO2 nanoparticles using simulated amorphisation and recrystallisation. Chemical Communications, 2004, , 2438.	2.2	84
69	Evolutionary techniques in atomistic simulation: thin films and nanoparticles. Current Opinion in Solid State and Materials Science, 2003, 7, 3-12.	5.6	22
70	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
71	Metal oxide encapsulated nanoparticles. Journal of Materials Chemistry, 2003, 13, 2078.	6.7	5
72	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

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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	Inducing Polycrystallinity within Supported Oxide Thin Films Using Template Buffer Layers. Journal of Physical Chemistry B, 2002, 106, 3778-3787.	1.2	10
75	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
76	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
77	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
78	Atomistic structure of oxide nanoparticles supported on an oxide substrate. Physical Review B, 2002, 65, .	1.1	24
79	Modelling oxide thin films. Molecular Simulation, 2002, 28, 683-725.	0.9	23
80	Structural exploration of thin-film oxide interfaces via â€˜simulated amorphisation and recrystallisationâ€™. Surface Science, 2001, 473, 97-107.	0.8	19
81	Evolution and atomistic structure of dislocations defects and clusters within CeO2 supported on ZrO2. Chemical Communications, 2001, , 289-290.	2.2	9
82	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
83	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
84	Simulated amorphisation and recrystallisation: nanocrystallites within meso-scale supported oxides. Journal of Materials Chemistry, 2000, 10, 2241-2243.	6.7	18
85	Atomistic simulation methodologies for modelling the nucleation, growth and structure of interfaces. Journal of Materials Chemistry, 2000, 10, 1315-1324.	6.7	24
86	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
87	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
88	The predicted 3-D atomistic structure of an interfacial screwâ€“edge dislocation. Journal of Materials Chemistry, 1999, 9, 2961-2964.	6.7	24
89	Strain reduction in supported materials; the formation of cracks and dislocations. Journal of Materials Chemistry, 1999, 9, 607-616.	6.7	6
90	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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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	An Introduction to Molecular Heterogeneous Catalysis. , 1998, , 189-214.		4
93	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
94	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
95	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
96	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
97	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
98	Computer Simulation of Structural, Defect and Surface Properties of Solids. , 1997, , 479-521.		2
99	Computer Modeling of the V2O5/TiO2Interface. The Journal of Physical Chemistry, 1996, 100, 8940-8945.	2.9	45
100	Computer modelling of V2O5: surface structures, crystal morphology and ethene sorption. Journal of Materials Chemistry, 1996, 6, 653.	6.7	26
101	Simulating the structures of crystals and their surfaces. Topics in Catalysis, 1996, 3, 135-167.	1.3	7
102	Sorption of ethene and ethane on the V2O5(001)/TiO2(001) anatase interface. Catalysis Letters, 1996, 38, 203-208.	1.4	9
103	Support Effect in V2o5 / Tio2 Partial Oxidation Catalysts. Oil & Gas Science & Technology, 1996, 51, 43-47.	0.2	2
104	Computer simulation study of the defect chemistry of rutile TiO2. Journal of Physics and Chemistry of Solids, 1995, 56, 799-805.	1.9	54
105	The stability of defects in the ceramic interfaces, and. Surface Science, 1995, 334, 170-178.	0.8	30
106	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
107	Effect of defects on the stability of heteroepitaxial ceramic interfaces studied by computer simulation. Physical Review B, 1994, 50, 14498-14505.	1.1	19
108	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

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109	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
110	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
111	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
112	Computer Simulation of Surface Segregation. Molecular Simulation, 1992, 9, 83-98.	0.9	27