Stephen A Shevlin

List of Publications by Year
in descending order

49 papers	8,032 citations	126858 33 h-index	189801 50 g-index
52 all docs	52 docs citations	52 times ranked	13438 citing authors

#	Article	IF	Citations
1	Computational materials design. Nature Materials, 2021, 20, 727-727.	13.3	10
2	A Metal-Free Oxygenated Covalent Triazine 2-D Photocatalyst Works Effectively from the Ultraviolet to Near-Infrared Spectrum for Water Oxidation Apart from Water Reduction. ACS Applied Energy Materials, 2020, 3, 8960-8968.	2.5	7
3	Unique hole-accepting carbon-dots promoting selective carbon dioxide reduction nearly 100% to methanol by pure water. Nature Communications, 2020, 11, 2531.	5.8	168
4	Towards rigorous multiscale flow models of nanoparticle reactivity in chemical looping applications. Catalysis Today, 2019, 338, 152-163.	2.2	7
5	Fast movement in a crowd. Nature Materials, 2019, 18, 431-431.	13.3	1
6	Efficient visible light-driven water oxidation and proton reduction by an ordered covalent triazine-based framework. Energy and Environmental Science, 2018, 11, 1617-1624.	15.6	212
7	Theory as a driving force to understand reactions on nanoparticles: general discussion. Faraday Discussions, 2018, 208, 147-185.	1.6	3
8	Highly crystallized Î±-FeOOH for a stable and efficient oxygen evolution reaction. Journal of Materials Chemistry A, 2017, 5, 2021-2028.	5.2	140
9	MOFs modeling and theory: general discussion. Faraday Discussions, 2017, 201, 233-245.	1.6	4
10	Electronic, magnetic and photophysical properties of MOFs and COFs: general discussion. Faraday Discussions, 2017, 201, 87-99.	1.6	9
11	Flexing with the flow. Nature Materials, 2017, 16, 785-785.	13.3	0
12	Nitrogen-Mediated Graphene Oxide Enables Highly Efficient Proton Transfer. Scientific Reports, 2017, 7, 5213.	1.6	4
13	Switching effective oxygen reduction and evolution performance by controlled graphitization of a cobaltâ€“nitrogenâ€“carbon framework system. Energy and Environmental Science, 2016, 9, 1661-1667.	15.6	281
14	Anionic Dopants for Improved Optical Absorption and Enhanced Photocatalytic Hydrogen Production in Graphitic Carbon Nitride. Chemistry of Materials, 2016, 28, 7250-7256.	3.2	39
15	Highly efficient rutile TiO₂ photocatalysts with single Cu(<scp>ii</scp>) and Fe(<scp>iii</scp>) surface catalytic sites. Journal of Materials Chemistry A, 2016, 4, 3127-3138.	5.2	73
16	Visible-light driven heterojunction photocatalysts for water splitting â€“ a critical review. Energy and Environmental Science, 2015, 8, 731-759.	15.6	1,985
17	Compressive Straining of Bilayer Phosphorene Leads to Extraordinary Electron Mobility at a New Conduction Band Edge. Nano Letters, 2015, 15, 2006-2010.	4.5	40
18	Polymorph Engineering of TiO₂: Demonstrating How Absolute Reference Potentials Are Determined by Local Coordination. Chemistry of Materials, 2015, 27, 3844-3851.	3.2	113

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19	Self-Energy Corrected <I>Ab Initio</I> Simulation of the Photo-Catalytic Material Nitrogen Doped Rutile TiO₂. Science of Advanced Materials, 2015, 7, 623-630.	0.1	4
20	Flexible and Binderâ€Free Organic Cathode for Highâ€Performance Lithiumâ€Ion Batteries. Advanced Materials, 2014, 26, 3338-3343.	11.1	200
21	Describing Excited State Relaxation and Localization in TiO₂ Nanoparticles Using TD-DFT. Journal of Chemical Theory and Computation, 2014, 10, 5538-5548.	2.3	34
22	Highly Efficient Photocatalytic H₂ Evolution from Water using Visible Light and Structureâ€Controlled Graphitic Carbon Nitride. Angewandte Chemie - International Edition, 2014, 53, 9240-9245.	7.2	1,000
23	Strain and Orientation Modulated Bandgaps and Effective Masses of Phosphorene Nanoribbons. Nano Letters, 2014, 14, 4607-4614.	4.5	306
24	Modeling Excited States in TiO₂ Nanoparticles: On the Accuracy of a TD-DFT Based Description. Journal of Chemical Theory and Computation, 2014, 10, 1189-1199.	2.3	63
25	Fe₂O₃â€“TiO₂ Nanocomposites for Enhanced Charge Separation and Photocatalytic Activity. Chemistry - A European Journal, 2014, 20, 15571-15579.	1.7	146
26	Limits to Doping of Wide Band Gap Semiconductors. Chemistry of Materials, 2013, 25, 2924-2926.	3.2	57
27	Band alignment of rutile and anatase TiO2. Nature Materials, 2013, 12, 798-801.	13.3	1,924
28	Accuracy of density functional theory in the prediction of carbon dioxide adsorbent materials. Dalton Transactions, 2013, 42, 4670.	1.6	15
29	MgH₂ Dehydrogenation Thermodynamics: Nanostructuring and Transition Metal Doping. Journal of Physical Chemistry C, 2013, 117, 10883-10891.	1.5	62
30	Structure and Defect Chemistry of Low- and High-Temperature Phases of LiBH₄. Journal of Physical Chemistry C, 2012, 116, 13488-13496.	1.5	25
31	High inertness of W@Si12 cluster toward O2 molecule. Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 376, 1454-1459.	0.9	6
32	Calcium-Based Functionalization of Carbon Materials for CO₂Capture: A First-Principles Computational Study. Journal of Physical Chemistry C, 2011, 115, 10990-10995.	1.5	51
33	Dehydrogenation mechanisms and thermodynamics of MNH2BH3 (M = Li, Na) metal amidoboranes as predicted from first principles. Physical Chemistry Chemical Physics, 2011, 13, 7649.	1.3	41
34	On the problem of cluster structure diversity and the value of data mining. Physical Chemistry Chemical Physics, 2010, 12, 8438.	1.3	30
35	Electronic and Optical Properties of Doped and Undoped (TiO₂)_n Nanoparticles. Journal of Physical Chemistry C, 2010, 114, 17333-17343.	1.5	101
36	First-principles study of the stability of calcium-decorated carbon nanostructures. Physical Review B, 2010, 82, .	1.1	53

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37	Advances in computational studies of energy materials. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2010, 368, 3379-3456.	1.6	119
38	Density functional theory simulations of complex hydride and carbon-based hydrogen storage materials. Chemical Society Reviews, 2009, 38, 211-225.	18.7	107
39	Construction of nano- and microporous frameworks from octahedral bubble clusters. Physical Chemistry Chemical Physics, 2009, 11, 3176.	1.3	34
40	Bubbles and microporous frameworks of silicon carbide. Physical Chemistry Chemical Physics, 2009, 11, 3186.	1.3	44
41	Multiscale simulation of onset plasticity during nanoindentation of Al (001) surface. Acta Materialia, 2008, 56, 4358-4368.	3.8	57
42	High-Capacity Room-Temperature Hydrogen Storage in Carbon Nanotubes via Defect-Modulated Titanium Doping. Journal of Physical Chemistry C, 2008, 112, 17456-17464.	1.5	71
43	Structure, optical properties and defects in nitride (IIIâ€“V) nanoscale cage clusters. Physical Chemistry Chemical Physics, 2008, 10, 1944.	1.3	42
44	Hydrogen-induced magnetization and tunable hydrogen storage in graphitic structures. Physical Review B, 2008, 77, .	1.1	33
45	Hydrogen sorption in defective hexagonal BN sheets and BN nanotubes. Physical Review B, 2007, 76, .	1.1	128
46	Transition-metal-doping-enhanced hydrogen storage in boron nitride systems. Applied Physics Letters, 2006, 89, 153104.	1.5	75
47	AbÂInitioDesign of High-kDielectrics:LaxY1â^'xAlO3. Physical Review Letters, 2005, 94, 146401.	2.9	47
48	Modeling of the Î²-SiC(001) (3Ã—2) surface reconstruction. Applied Surface Science, 2000, 162-163, 94-99.	3.1	5
49	Modeling thec(4Ã—2)reconstruction ofÎ²â^'SiC(001). Physical Review B, 2000, 62, 6904-6907.	1.1	11