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	Visible-light driven heterojunction photocatalysts for water splitting â€“ a critical review. Energy and Environmental Science, 2015, 8, 731-759.	15.6	1,985
2	Band alignment of rutile and anatase TiO2. Nature Materials, 2013, 12, 798-801.	13.3	1,924
3	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
4	Strain and Orientation Modulated Bandgaps and Effective Masses of Phosphorene Nanoribbons. Nano Letters, 2014, 14, 4607-4614.	4.5	306
5	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
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	Flexible and Binderâ€Free Organic Cathode for Highâ€Performance Lithiumâ€Ion Batteries. Advanced Materials, 2014, 26, 3338-3343.	11.1	200
8	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
9	Fe₂O₃â€“TiO₂ Nanocomposites for Enhanced Charge Separation and Photocatalytic Activity. Chemistry - A European Journal, 2014, 20, 15571-15579.	1.7	146
10	Highly crystallized Î±-FeOOH for a stable and efficient oxygen evolution reaction. Journal of Materials Chemistry A, 2017, 5, 2021-2028.	5.2	140
11	Hydrogen sorption in defective hexagonal BN sheets and BN nanotubes. Physical Review B, 2007, 76, .	1.1	128
12	Advances in computational studies of energy materials. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2010, 368, 3379-3456.	1.6	119
13	Polymorph Engineering of TiO₂: Demonstrating How Absolute Reference Potentials Are Determined by Local Coordination. Chemistry of Materials, 2015, 27, 3844-3851.	3.2	113
14	Density functional theory simulations of complex hydride and carbon-based hydrogen storage materials. Chemical Society Reviews, 2009, 38, 211-225.	18.7	107
15	Electronic and Optical Properties of Doped and Undoped (TiO₂)_n Nanoparticles. Journal of Physical Chemistry C, 2010, 114, 17333-17343.	1.5	101
16	Transition-metal-doping-enhanced hydrogen storage in boron nitride systems. Applied Physics Letters, 2006, 89, 153104.	1.5	75
17	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
18	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

#	Article	IF	Citations
19	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
20	MgH₂ Dehydrogenation Thermodynamics: Nanostructuring and Transition Metal Doping. Journal of Physical Chemistry C, 2013, 117, 10883-10891.	1.5	62
21	Multiscale simulation of onset plasticity during nanoindentation of Al (001) surface. Acta Materialia, 2008, 56, 4358-4368.	3.8	57
22	Limits to Doping of Wide Band Gap Semiconductors. Chemistry of Materials, 2013, 25, 2924-2926.	3.2	57
23	First-principles study of the stability of calcium-decorated carbon nanostructures. Physical Review B, 2010, 82, .	1.1	53
24	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
25	AbÂInitioDesign of High-kDielectrics:LaxY1â˜'xAlO3. Physical Review Letters, 2005, 94, 146401.	2.9	47
26	Bubbles and microporous frameworks of silicon carbide. Physical Chemistry Chemical Physics, 2009, 11, 3186.	1.3	44
27	Structure, optical properties and defects in nitride (IIIâ€“V) nanoscale cage clusters. Physical Chemistry Chemical Physics, 2008, 10, 1944.	1.3	42
28	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
29	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
30	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
31	Construction of nano- and microporous frameworks from octahedral bubble clusters. Physical Chemistry Chemical Physics, 2009, 11, 3176.	1.3	34
32	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
33	Hydrogen-induced magnetization and tunable hydrogen storage in graphitic structures. Physical Review B, 2008, 77, .	1.1	33
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	Structure and Defect Chemistry of Low- and High-Temperature Phases of LiBH₄. Journal of Physical Chemistry C, 2012, 116, 13488-13496.	1.5	25
36	Accuracy of density functional theory in the prediction of carbon dioxide adsorbent materials. Dalton Transactions, 2013, 42, 4670.	1.6	15

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37	Modeling thec(4Ã—2)reconstruction ofÎ²â^'SiC(001). Physical Review B, 2000, 62, 6904-6907.	1.1	11
38	Computational materials design. Nature Materials, 2021, 20, 727-727.	13.3	10
39	Electronic, magnetic and photophysical properties of MOFs and COFs: general discussion. Faraday Discussions, 2017, 201, 87-99.	1.6	9
40	Towards rigorous multiscale flow models of nanoparticle reactivity in chemical looping applications. Catalysis Today, 2019, 338, 152-163.	2.2	7
41	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
42	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
43	Modeling of the Î²-SiC(001) (3Ã—2) surface reconstruction. Applied Surface Science, 2000, 162-163, 94-99.	3.1	5
44	MOFs modeling and theory: general discussion. Faraday Discussions, 2017, 201, 233-245.	1.6	4
45	Nitrogen-Mediated Graphene Oxide Enables Highly Efficient Proton Transfer. Scientific Reports, 2017, 7, 5213.	1.6	4
46	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
47	Theory as a driving force to understand reactions on nanoparticles: general discussion. Faraday Discussions, 2018, 208, 147-185.	1.6	3
48	Fast movement in a crowd. Nature Materials, 2019, 18, 431-431.	13.3	1
49	Flexing with the flow. Nature Materials, 2017, 16, 785-785.	13.3	0