Sean C Smith

List of Publications by Citations

353 papers	21,299 citations	62 h-index	136 g-index
368 ext. papers	23,624 ext. citations	6.7 avg, IF	7.01 L-index

#	Paper	IF	Citations
353	Anatase TiO2 single crystals with a large percentage of reactive facets. *Nature*, **2008**, 453, 638-41	50.4	3391
352	Unique electronic structure induced high photoreactivity of sulfur-doped graphitic C3N4. *Journal of the American Chemical Society*, **2010**, 132, 11642-8	16.4	1597
351	Solvothermal synthesis and photoreactivity of anatase TiO(2) nanosheets with dominant {001} facets. *Journal of the American Chemical Society*, **2009**, 131, 4078-83	16.4	1149
350	Nanoporous graphitic-C3N4@carbon metal-free electrocatalysts for highly efficient oxygen reduction. *Journal of the American Chemical Society*, **2011**, 133, 20116-9	16.4	869
349	Phosphorene: Fabrication, Properties, and Applications. *Journal of Physical Chemistry Letters*, **2015**, 6, 2794-805	6.4	545
348	Hybrid graphene and graphitic carbon nitride nanocomposite: gap opening, electron-hole puddle, interfacial charge transfer, and enhanced visible light response. *Journal of the American Chemical Society*, **2012**, 134, 4393-7	16.4	490
347	Isolated Diatomic Ni-Fe Metal-Nitrogen Sites for Synergistic Electroreduction of CO. *Angewandte Chemie - International Edition*, **2019**, 58, 6972-6976	16.4	406
346	Understanding the Enhancement in Photoelectrochemical Properties of Photocatalytically Prepared TiO2-Reduced Graphene Oxide Composite. *Journal of Physical Chemistry C*, **2011**, 115, 6004-6009	3.8	377
345	Nanosized anatase TiO2 single crystals for enhanced photocatalytic activity. *Chemical Communications*, **2010**, 46, 755-7	5.8	375
344	Graphdiyne: a versatile nanomaterial for electronics and hydrogen purification. *Chemical Communications*, **2011**, 47, 11843-5	5.8	289
343	Multifunctional porous graphene for nanoelectronics and hydrogen storage: new properties revealed by first principle calculations. *Journal of the American Chemical Society*, **2010**, 132, 2876-7	16.4	277
342	Band-to-Band Visible-Light Photon Excitation and Photoactivity Induced by Homogeneous Nitrogen Doping in Layered Titanates. *Chemistry of Materials*, **2009**, 21, 1266-1274	9.6	259
341	First-principles prediction of metal-free magnetism and intrinsic half-metallicity in graphitic carbon nitride. *Physical Review Letters*, **2012**, 108, 197207	7.4	234
340	Hybrid Graphene/Titania Nanocomposite: Interface Charge Transfer, Hole Doping, and Sensitization for Visible Light Response. *Journal of Physical Chemistry Letters*, **2011**, 2, 894-9	6.4	230
339	Titania-water interactions: a review of theoretical studies. *Journal of Materials Chemistry*, **2010**, 20, 10319		228
338	Higher charge/discharge rates of lithium-ions across engineered TiO2 surfaces leads to enhanced battery performance. *Chemical Communications*, **2010**, 46, 6129-31	5.8	197
337	Structural and Electronic Properties of Layered Arsenic and Antimony Arsenide. *Journal of Physical Chemistry C*, **2015**, 119, 6918-6922	3.8	184

336	Single Mo1(Cr1) Atom on Nitrogen-Doped Graphene Enables Highly Selective Electroreduction of Nitrogen into Ammonia. *ACS Catalysis*, **2019**, 9, 3419-3425	13.1	170
335	Dots versus antidots: computational exploration of structure, magnetism, and half-metallicity in boron-nitride nanostructures. *Journal of the American Chemical Society*, **2009**, 131, 17354-9	16.4	158
334	First-principle studies of electronic structure and C-doping effect in boron nitride nanoribbon. *Chemical Physics Letters*, **2007**, 447, 181-186	2.5	158
333	Ultrasmall Water-Soluble and Biocompatible Magnetic Iron Oxide Nanoparticles as Positive and Negative Dual Contrast Agents. *Advanced Functional Materials*, **2012**, 22, 2387-2393	15.6	155
332	Lithium-Catalyzed Dehydrogenation of Ammonia Borane within Mesoporous Carbon Framework for Chemical Hydrogen Storage. *Advanced Functional Materials*, **2009**, 19, 265-271	15.6	148
331	Bond selection in the photoisomerization reaction of anionic green fluorescent protein and kindling fluorescent protein chromophore models. *Journal of the American Chemical Society*, **2008**, 130, 8677-89	16.4	135
330	Boosting Oxygen Evolution Reaction by Creating Both Metal Ion and Lattice-Oxygen Active Sites in a Complex Oxide. *Advanced Materials*, **2020**, 32, e1905025	24	122
329	N-Doped CsTaWO6 as a New Photocatalyst for Hydrogen Production from Water Splitting Under Solar Irradiation. *Advanced Functional Materials*, **2011**, 21, 126-132	15.6	120
328	High activity and durability of novel perovskite electrocatalysts for water oxidation. *Materials Horizons*, **2015**, 2, 495-501	14.4	119
327	Iodine doped anatase TiO2 photocatalyst with ultra-long visible light response: correlation between geometric/electronic structures and mechanisms. *Journal of Materials Chemistry*, **2009**, 19, 2822		119
326	Surface-induced orientation control of CuPc molecules for the epitaxial growth of highly ordered organic crystals on graphene. *Journal of the American Chemical Society*, **2013**, 135, 3680-7	16.4	117
325	Unusual synergistic effect in layered Ruddlesden-Popper oxide enables ultrafast hydrogen evolution. *Nature Communications*, **2019**, 10, 149	17.4	116
324	Metallic and carbon nanotube-catalyzed coupling of hydrogenation in magnesium. *Journal of the American Chemical Society*, **2007**, 129, 15650-4	16.4	114
323	Efficient Promotion of Anatase TiO2 Photocatalysis via Bifunctional Surface-Terminating TiOBN Structures. *Journal of Physical Chemistry C*, **2009**, 113, 12317-12324	3.8	109
322	Photodissociation of benzene under collision-free conditions: an ab initio/Rice-Ramsperger-Kassel-Marcus study. *Journal of Chemical Physics*, **2004**, 120, 7008-17	3.9	107
321	A Janus MoSSe monolayer: a superior and strain-sensitive gas sensing material. *Journal of Materials Chemistry A*, **2019**, 7, 1099-1106	13	106
320	Quantum spin Hall effect and topological phase transition in two-dimensional square transition-metal dichalcogenides. *Physical Review B*, **2015**, 92,	3.3	106
319	Sulfur doped anatase TiO2 single crystals with a high percentage of {0 0 1} facets. *Journal of Colloid and Interface Science*, **2010**, 349, 477-83	9.3	103

318	C-BN single-walled nanotubes from hybrid connection of BN/C nanoribbons: prediction by ab initio density functional calculations. *Journal of the American Chemical Society*, **2009**, 131, 1682-3	16.4	100
317	The role of Ti as a catalyst for the dissociation of hydrogen on a Mg(0001) surface. *Journal of Physical Chemistry B*, **2005**, 109, 18037-41	3.4	100
316	Hydrogen spillover mechanism on a Pd-doped Mg surface as revealed by ab initio density functional calculation. *Journal of the American Chemical Society*, **2007**, 129, 10201-4	16.4	94
315	Hydrogen Incorporation and Storage in Well-Defined Nanocrystals of Anatase Titanium Dioxide. *Journal of Physical Chemistry C*, **2011**, 115, 25590-25594	3.8	92
314	The calculation of vibrational eigenstates by MINRES filter diagonalization. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1997**, 101, 400-406		92
313	Anisotropic Ripple Deformation in Phosphorene. *Journal of Physical Chemistry Letters*, **2015**, 6, 1509-13	6.4	88
312	New Family of Quantum Spin Hall Insulators in Two-dimensional Transition-Metal Halide with Large Nontrivial Band Gaps. *Nano Letters*, **2015**, 15, 7867-72	11.5	87
311	Modelling carbon membranes for gas and isotope separation. *Physical Chemistry Chemical Physics*, **2013**, 15, 4832-43	3.6	84
310	First principle studies of zigzag AlN nanoribbon. *Chemical Physics Letters*, **2009**, 469, 183-185	2.5	83
309	The isotopic effects of deuteration on optoelectronic properties of conducting polymers. *Nature Communications*, **2014**, 5, 3180	17.4	82
308	Mg-based nanocomposites with high capacity and fast kinetics for hydrogen storage. *Journal of Physical Chemistry B*, **2006**, 110, 11697-703	3.4	80
307	Electroreduction of CO2 to CO on a Mesoporous Carbon Catalyst with Progressively Removed Nitrogen Moieties. *ACS Energy Letters*, **2018**, 3, 2292-2298	20.1	78
306	Photocatalytic Hydrogen Production from Water Using N-Doped Ba5Ta4O15 under Solar Irradiation. *Journal of Physical Chemistry C*, **2011**, 115, 15674-15678	3.8	77
305	State-to-state reactive differential cross sections for the H+H2-->H2+H reaction on five different potential energy surfaces employing a new quantum wavepacket computer code: DIFFREALWAVE. *Journal of Chemical Physics*, **2006**, 125, 164303	3.9	77
304	A density functional theory study on CO2 capture and activation by graphene-like boron nitride with boron vacancy. *Catalysis Today*, **2011**, 175, 271-275	5.3	74
303	Angular momentum conservation in unimolecular and recombination reactions. *International Journal of Chemical Kinetics*, **1988**, 20, 307-329	1.4	74
302	Processable Surface Modification of Nickel-Heteroatom (N, S) Bridge Sites for Promoted Alkaline Hydrogen Evolution. *Angewandte Chemie - International Edition*, **2019**, 58, 461-466	16.4	74
301	Radiationless decay of red fluorescent protein chromophore models via twisted intramolecular charge-transfer states. *Journal of the American Chemical Society*, **2007**, 129, 2054-65	16.4	73

300	The 2.1A crystal structure of the far-red fluorescent protein HcRed: inherent conformational flexibility of the chromophore. *Journal of Molecular Biology*, **2005**, 349, 223-37	6.5	73
299	Direct insights into the role of epoxy groups on cobalt sites for acidic HO production. *Nature Communications*, **2020**, 11, 4181	17.4	73
298	Extraordinary water adsorption characteristics of graphene oxide. *Chemical Science*, **2018**, 9, 5106-5111	9.4	72
297	The effect of pH on PAMAM dendrimer-siRNA complexation: endosomal considerations as determined by molecular dynamics simulation. *Biophysical Chemistry*, **2011**, 158, 126-33	3.5	70
296	Asymmetrically Decorated, Doped Porous Graphene As an Effective Membrane for Hydrogen Isotope Separation. *Journal of Physical Chemistry C*, **2012**, 116, 6672-6676	3.8	69
295	Synthesis and Biological Activity Of Unsymmetrical Bis-Steroidal Pyrazines Related to the Cytotoxic Marine Natural Product Cephalostatin 1. *Journal of Organic Chemistry*, **1994**, 59, 6828-6839	4.2	67
294	Formation and Migration of Oxygen Vacancies in SrCoO3 and Their Effect on Oxygen Evolution Reactions. *ACS Catalysis*, **2016**, 6, 5565-5570	13.1	66
293	Implanting Ni-O-VOx sites into Cu-doped Ni for low-overpotential alkaline hydrogen evolution. *Nature Communications*, **2020**, 11, 2720	17.4	65
292	Borophene as a Promising Material for Charge-Modulated Switchable CO Capture. *ACS Applied Materials & Interfaces*, **2017**, 9, 19825-19830	9.5	62
291	Preparation of new sulfur-doped and sulfur/nitrogen co-doped CsTaWO6 photocatalysts for hydrogen production from water under visible light. *Journal of Materials Chemistry*, **2011**, 21, 8871		60
290	Nitrogen doping in ion-exchangeable layered tantalate towards visible-light induced water oxidation. *Chemical Communications*, **2011**, 47, 6293-5	5.8	57
289	Statistical modeling of ion□molecule electrostatic capture. *Journal of Chemical Physics*, **1992**, 97, 5451-5464	3.9	57
288	H2 purification by functionalized graphdiyne □role of nitrogen doping. *Journal of Materials Chemistry A*, **2015**, 3, 6767-6771	13	56
287	Phosphine vapor-assisted construction of heterostructured Ni2P/NiTe2 catalysts for efficient hydrogen evolution. *Energy and Environmental Science*, **2020**, 13, 1799-1807	35.4	56
286	Interfacing BiVO with Reduced Graphene Oxide for Enhanced Photoactivity: A Tale of Facet Dependence of Electron Shuttling. *Small*, **2016**, 12, 5295-5302	11	56
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282	On the microscopic mechanism of carbon gasification: A theoretical study. *Carbon*, **2004**, 42, 2921-2928	10.4	55
281	The relationship between recombination, chemical activation and unimolecular dissociation rate coefficients. *Journal of Chemical Physics*, **1989**, 90, 4265-4273	3.9	55
280	A density functional theory study of CO2 and N2 adsorption on aluminium nitride single walled nanotubes. *Journal of Materials Chemistry*, **2010**, 20, 10426		54
279	p-Doped Graphene/Graphitic Carbon Nitride Hybrid Electrocatalysts: Unraveling Charge Transfer Mechanisms for Enhanced Hydrogen Evolution Reaction Performance. *ACS Catalysis*, **2016**, 6, 7071-7077	13.1	53
278	Electronic Functionality in Graphene-Based Nanoarchitectures: Discovery and Design via First-Principles Modeling. *Journal of Physical Chemistry Letters*, **2011**, 2, 73-80	6.4	53
277	The controlled disassembly of mesostructured perovskites as an avenue to fabricating high performance nanohybrid catalysts. *Nature Communications*, **2017**, 8, 15553	17.4	52
276	On the mechanism of gas adsorption for pristine, defective and functionalized graphene. *Physical Chemistry Chemical Physics*, **2017**, 19, 6051-6056	3.6	51
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274	N,P co-coordinated Fe species embedded in carbon hollow spheres for oxygen electrocatalysis. *Journal of Materials Chemistry A*, **2019**, 7, 14732-14742	13	50
273	Convergent proton-transfer photocycles violate mirror-image symmetry in a key melanin monomer. *Journal of the American Chemical Society*, **2007**, 129, 6672-3	16.4	50
272	Surface Reconstruction of Ultrathin Palladium Nanosheets during Electrocatalytic CO Reduction. *Angewandte Chemie - International Edition*, **2020**, 59, 21493-21498	16.4	50
271	Single-phase perovskite oxide with super-exchange induced atomic-scale synergistic active centers enables ultrafast hydrogen evolution. *Nature Communications*, **2020**, 11, 5657	17.4	49
270	Conductive Graphitic Carbon Nitride as an Ideal Material for Electrocatalytically Switchable CO2 Capture. *Scientific Reports*, **2015**, 5, 17636	4.9	48
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268	First-principle study of adsorption of hydrogen on Ti-doped Mg(0001) surface. *Journal of Physical Chemistry B*, **2006**, 110, 21747-50	3.4	48
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265	Adsorption of Carbon Dioxide and Nitrogen on Single-Layer Aluminum Nitride Nanostructures Studied by Density Functional Theory. *Journal of Physical Chemistry C*, **2010**, 114, 7846-7849	3.8	46

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263	Role of charge in destabilizing AlH4 and BH4 complex anions for hydrogen storage applications: Ab initio density functional calculations. *Physical Review B*, **2006**, 74,	3.3	45
262	Structure, dynamics, and energetics of siRNA-cationic vector complexation: a molecular dynamics study. *Journal of Physical Chemistry B*, **2010**, 114, 9220-30	3.4	44
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260	Angular-momentum resolution in transitional-mode state counting for loose transition states. *Journal of Chemical Physics*, **1992**, 97, 2406-2416	3.9	44
259	Super-Exchange Interaction Induced Overall Optimization in Ferromagnetic Perovskite Oxides Enables Ultrafast Water Oxidation. *Small*, **2019**, 15, e1903120	11	43
258	Lattice distortion oriented angular self-assembly of monolayer titania sheets. *Journal of the American Chemical Society*, **2011**, 133, 695-7	16.4	43
257	The dynamics of the H(+) + D(2) reaction: a comparison of quantum mechanical wavepacket, quasi-classical and statistical-quasi-classical results. *Physical Chemistry Chemical Physics*, **2010**, 12, 1102-15	3.6	43
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255	Isolated Diatomic Ni-Fe Metal–Nitrogen Sites for Synergistic Electroreduction of CO2. *Angewandte Chemie*, **2019**, 131, 7046-7050	3.6	42
254	Full Iterative Solution of the Two-Dimensional Master Equation for Thermal Unimolecular Reactions. *The Journal of Physical Chemistry*, **1996**, 100, 7090-7096		42
253	Structure and dynamics of multiple cationic vectors-siRNA complexation by all-atomic molecular dynamics simulations. *Journal of Physical Chemistry B*, **2010**, 114, 9231-7	3.4	41
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251	Conductive Boron-Doped Graphene as an Ideal Material for Electrocatalytically Switchable and High-Capacity Hydrogen Storage. *ACS Applied Materials & Interfaces*, **2016**, 8, 32815-32822	9.5	40
250	Kinetic isotope effect for ground state proton transfer in the green fluorescent protein: a quantum-kinetic model. *Physical Chemistry Chemical Physics*, **2009**, 11, 8422-4	3.6	40
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248	Entropy barriers to proton transfer. *Journal of the American Chemical Society*, **1991**, 113, 862-869	16.4	39
247	Intercalation of Sulfonate into Layered Double Hydroxide: Comparison of Simulation with Experiment. *Journal of Physical Chemistry C*, **2009**, 113, 559-566	3.8	38

246	Atomically Dispersed Indium Sites for Selective CO Electroreduction to Formic Acid. *ACS Nano*, **2021**, 15, 5671-5678	16.7	38
245	Layered Graphene-Hexagonal BN Nanocomposites: Experimentally Feasible Approach to Charge-Induced Switchable CO2 Capture. *ChemSusChem*, **2015**, 8, 2987-93	8.3	37
244	DIFFREALWAVE: A parallel real wavepacket code for the quantum mechanical calculation of reactive state-to-state differential cross sections in atom plus diatom collisions. *Computer Physics Communications*, **2008**, 179, 569-578	4.2	37
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238	Unimolecular decomposition of a polyatomic ion in a variable-temperature selected-ion-flow-drift tube: experiment and theoretical interpretation. *International Journal of Mass Spectrometry and Ion Processes*, **1990**, 96, 77-96		35
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236	Synthesis and Characterization of Colloidal Core–Shell Semiconductor Nanowires. *European Journal of Inorganic Chemistry*, **2010**, 2010, 4325-4331	2.3	34
235	Microscopic rate coefficients in reactions with flexible transition states: Analysis of the transitional-mode sum of states. *Journal of Chemical Physics*, **1991**, 95, 3404-3430	3.9	34
234	Angular momentum conservation in multichannel unimolecular reactions. *International Journal of Chemical Kinetics*, **1988**, 20, 979-990	1.4	34
233	Theoretical Predictions of Freestanding Honeycomb Sheets of Cadmium Chalcogenides. *Journal of Physical Chemistry C*, **2014**, 118, 16236-16245	3.8	33
232	A formation mechanism of oxygen vacancies in a MnO2 monolayer: a DFT + U study. *Physical Chemistry Chemical Physics*, **2011**, 13, 11325-8	3.6	33
231	Integral and differential cross sections for the S(1D)+HD reaction employing the ground adiabatic electronic state. *Physical Chemistry Chemical Physics*, **2009**, 11, 11587-95	3.6	33
230	Pyrite-type ruthenium disulfide with tunable disorder and defects enables ultra-efficient overall water splitting. *Journal of Materials Chemistry A*, **2019**, 7, 14222-14232	13	32
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227	Half metallicty in finite-length zigzag single walled carbon nanotube: A first-principle prediction. *Applied Physics Letters*, **2008**, 93, 073101	3.4	31
226	Efficient time-independent wave packet scattering calculations within a Lanczos subspace: H+O2 (J=0) state-to-state reaction probabilities. *Journal of Chemical Physics*, **2002**, 116, 2354-2360	3.9	31
225	Variational transition state theory: a simple model for dissociation and recombination reactions of small species. *The Journal of Physical Chemistry*, **1991**, 95, 8685-8694		31
224	Understanding the high activity of mildly reduced graphene oxide electrocatalysts in oxygen reduction to hydrogen peroxide. *Materials Horizons*, **2019**, 6, 1409-1415	14.4	30
223	Just add sugar for´carbohydrate induced self-assembly of curcumin. *Nature Communications*, **2019**, 10, 582	17.4	30
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206	Tungsten Oxide/Carbide Surface Heterojunction Catalyst with High Hydrogen Evolution Activity. *ACS Energy Letters*, **2020**, 5, 3560-3568	20.1	27
205	Confinement of Ionic Liquids at Single-Ni-Sites Boost Electroreduction of CO2 in Aqueous Electrolytes. *ACS Catalysis*, **2020**, 10, 13171-13178	13.1	27
204	Light-Induced Synergistic Multidefect Sites on TiO2/SiO2 Composites for Catalytic Dehydrogenation. *ACS Catalysis*, **2019**, 9, 2674-2684	13.1	27
203	Antipoisoning Nickel□arbon Electrocatalyst for Practical Electrochemical CO2 Reduction to CO. *ACS Applied Energy Materials*, **2019**, 2, 8002-8009	6.1	26
202	Exceptional Optoelectronic Properties of Hydrogenated Bilayer Silicene. *Physical Review X*, **2014**, 4,	9.1	26
201	OH-initiated oxidation of toluene. 1. Quantum chemistry investigation of the reaction path. *Journal of Physical Chemistry A*, **2007**, 111, 3686-90	2.8	26
200	Production and loss of HC3N in interstellar clouds: some relevant laboratory measurements. *Monthly Notices of the Royal Astronomical Society*, **1986**, 219, 89-94	4.3	26
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197	Temperature Dependence of Rate Coefficients and Branching Ratios for the NH2 + NO Reaction via Microcanonical Variational Transition State Theory. *The Journal of Physical Chemistry*, **1996**, 100, 12349-12354		25
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195	Converged quantum calculations of HO2 bound states and resonances for J=6 and 10. *Journal of Chemical Physics*, **2004**, 120, 9583-93	3.9	24
194	Intrinsic ORR Activity Enhancement of Pt Atomic Sites by Engineering the d-Band Center via Local Coordination Tuning. *Angewandte Chemie - International Edition*, **2021**, 60, 21911-21917	16.4	24
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List of Publications

12	Bridge- and Double-Bonded O and NH on Fully OH- and NH2-Terminated Silicon Nanocrystals: Ground and Excited State Properties (Phys. Status Solidi B 5/2019). *Physica Status Solidi (B): Basic Research*, **2019**, 256, 1970023	1.3
11	Cell Membrane Penetration without Pore Formation: Chameleonic Properties of Dendrimers in Response to Hydrophobic and Hydrophilic Environments. *Advanced Theory and Simulations*, **2020**, 3, 1900152	3.5
10	Molecular Modeling of Layered Double Hydroxide Nanoparticles for Drug Delivery **2015**, 197-216	
9	Colloidal Semiconductor Nanowires **2013**, 65-104	
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6	Unimolecular Reaction Dynamics: Theory and Experiments (Baer, Tomas; Hase, William L.). *Journal of Chemical Education*, **1998**, 75, 1098	2.4
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4	Hexagonal honeycomb silicon: Silicene. *Series in Materials Science and Engineering*, **2017**, 171-188	
3	Design guidelines for transition metals as interstitial emitters in silicon nanocrystals to tune photoluminescence properties: zinc as biocompatible example. *Nanoscale*, **2020**, 12, 19340-19349	7.7
2	On the Location of Boron in SiO2-Embedded Si Nanocrystals: An X-ray Absorption Spectroscopy and Density Functional Theory Study. *Physica Status Solidi (B): Basic Research*, **2021**, 258, 2000623	1.3
1	Photocatalysis: Interfacing BiVO4 with Reduced Graphene Oxide for Enhanced Photoactivity: A Tale of Facet Dependence of Electron Shuttling (Small 38/2016). *Small*, **2016**, 12, 5232-5232	11