Sean C Smith

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5114658/publications.pdf

Version: 2024-02-01

		9234	7496
353	26,200	74	151
papers	citations	h-index	g-index

368	368	368	25833
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Anatase TiO2 single crystals with a large percentage of reactive facets. Nature, 2008, 453, 638-641.	13.7	3,753
2	Unique Electronic Structure Induced High Photoreactivity of Sulfur-Doped Graphitic C₃N₄. Journal of the American Chemical Society, 2010, 132, 11642-11648.	6.6	1,856
3	Solvothermal Synthesis and Photoreactivity of Anatase TiO₂ Nanosheets with Dominant {001} Facets. Journal of the American Chemical Society, 2009, 131, 4078-4083.	6.6	1,237
4	Nanoporous Graphitic-C₃N₄@Carbon Metal-Free Electrocatalysts for Highly Efficient Oxygen Reduction. Journal of the American Chemical Society, 2011, 133, 20116-20119.	6.6	958
5	Isolated Diatomic Niâ€Fe Metalâ€“Nitrogen Sites for Synergistic Electroreduction of CO₂. Angewandte Chemie - International Edition, 2019, 58, 6972-6976.	7.2	707
6	Phosphorene: Fabrication, Properties, and Applications. Journal of Physical Chemistry Letters, 2015, 6, 2794-2805.	2.1	680
7	Hybrid Graphene and Graphitic Carbon Nitride Nanocomposite: Gap Opening, Electronâ€“Hole Puddle, Interfacial Charge Transfer, and Enhanced Visible Light Response. Journal of the American Chemical Society, 2012, 134, 4393-4397.	6.6	565
8	Nanosized anatase TiO2 single crystals for enhanced photocatalytic activity. Chemical Communications, 2010, 46, 755-757.	2.2	403
9	Understanding the Enhancement in Photoelectrochemical Properties of Photocatalytically Prepared TiO₂-Reduced Graphene Oxide Composite. Journal of Physical Chemistry C, 2011, 115, 6004-6009.	1.5	403
10	Graphdiyne: a versatile nanomaterial for electronics and hydrogen purification. Chemical Communications, 2011, 47, 11843.	2.2	329
11	Multifunctional Porous Graphene for Nanoelectronics and Hydrogen Storage: New Properties Revealed by First Principle Calculations. Journal of the American Chemical Society, 2010, 132, 2876-2877.	6.6	304
12	Band-to-Band Visible-Light Photon Excitation and Photoactivity Induced by Homogeneous Nitrogen Doping in Layered Titanates. Chemistry of Materials, 2009, 21, 1266-1274.	3.2	284
13	First-Principles Prediction of Metal-Free Magnetism and Intrinsic Half-Metallicity in Graphitic Carbon Nitride. Physical Review Letters, 2012, 108, 197207.	2.9	272
14	Single Mo₁(Cr₁) Atom on Nitrogen-Doped Graphene Enables Highly Selective Electroreduction of Nitrogen into Ammonia. ACS Catalysis, 2019, 9, 3419-3425.	5.5	258
15	Titania-water interactions: a review of theoretical studies. Journal of Materials Chemistry, 2010, 20, 10319.	6.7	255
16	Hybrid Graphene/Titania Nanocomposite: Interface Charge Transfer, Hole Doping, and Sensitization for Visible Light Response. Journal of Physical Chemistry Letters, 2011, 2, 894-899.	2.1	252
17	Higher charge/discharge rates of lithium-ions across engineered TiO2 surfaces leads to enhanced battery performance. Chemical Communications, 2010, 46, 6129.	2.2	216
18	Structural and Electronic Properties of Layered Arsenic and Antimony Arsenide. Journal of Physical Chemistry C, 2015, 119, 6918-6922.	1.5	210

#	Article	IF	Citations
19	Direct insights into the role of epoxy groups on cobalt sites for acidic H2O2 production. Nature Communications, 2020, 11, 4181.	5.8	204
20	Boosting Oxygen Evolution Reaction by Creating Both Metal Ion and Latticeâ€Oxygen Active Sites in a Complex Oxide. Advanced Materials, 2020, 32, e1905025.	11.1	190
21	Unusual synergistic effect in layered Ruddlesdenâ^'Popper oxide enables ultrafast hydrogen evolution. Nature Communications, 2019, 10, 149.	5.8	187
22	A Janus MoSSe monolayer: a superior and strain-sensitive gas sensing material. Journal of Materials Chemistry A, 2019, 7, 1099-1106.	5.2	187
23	Ultrasmall Waterâ€Soluble and Biocompatible Magnetic Iron Oxide Nanoparticles as Positive and Negative Dual Contrast Agents. Advanced Functional Materials, 2012, 22, 2387-2393.	7.8	181
24	First-principle studies of electronic structure and C-doping effect in boron nitride nanoribbon. Chemical Physics Letters, 2007, 447, 181-186.	1.2	180
25	Dots versus Antidots: Computational Exploration of Structure, Magnetism, and Half-Metallicity in Boronâ^'Nitride Nanostructures. Journal of the American Chemical Society, 2009, 131, 17354-17359.	6.6	174
26	Lithiumâ€Catalyzed Dehydrogenation of Ammonia Borane within Mesoporous Carbon Framework for Chemical Hydrogen Storage. Advanced Functional Materials, 2009, 19, 265-271.	7.8	156
27	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, 8677-8689.	6.6	149
28	Nâ€Doped CsTaWO₆ as a New Photocatalyst for Hydrogen Production from Water Splitting Under Solar Irradiation. Advanced Functional Materials, 2011, 21, 126-132.	7.8	135
29	Single-phase perovskite oxide with super-exchange induced atomic-scale synergistic active centers enables ultrafast hydrogen evolution. Nature Communications, 2020, 11, 5657.	5.8	134
30	Photodissociation of benzene under collision-free conditions: An ab initio/Riceâ€“Ramspergerâ€“Kasselâ€“Marcus study. Journal of Chemical Physics, 2004, 120, 7008-7017.	1.2	133
31	A single-Pt-atom-on-Ru-nanoparticle electrocatalyst for CO-resilient methanol oxidation. Nature Catalysis, 2022, 5, 231-237.	16.1	133
32	Intrinsic ORR Activity Enhancement of Pt Atomic Sites by Engineering the dâ€Band Center via Local Coordination Tuning. Angewandte Chemie - International Edition, 2021, 60, 21911-21917.	7.2	132
33	Metallic and Carbon Nanotube-Catalyzed Coupling of Hydrogenation in Magnesium. Journal of the American Chemical Society, 2007, 129, 15650-15654.	6.6	131
34	Electroreduction of CO₂ to CO on a Mesoporous Carbon Catalyst with Progressively Removed Nitrogen Moieties. ACS Energy Letters, 2018, 3, 2292-2298.	8.8	129
35	High activity and durability of novel perovskite electrocatalysts for water oxidation. Materials Horizons, 2015, 2, 495-501.	6.4	128
36	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.	6.7	127

#	Article	IF	Citations
37	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, 3680-3687.	6.6	125
38	Atomically Dispersed Indium Sites for Selective CO₂ Electroreduction to Formic Acid. ACS Nano, 2021, 15, 5671-5678.	7.3	121
39	Isolated copperâ€“tin atomic interfaces tuning electrocatalytic CO2 conversion. Nature Communications, 2021, 12, 1449.	5.8	119
40	Quantum spin Hall effect and topological phase transition in two-dimensional square transition-metal dichalcogenides. Physical Review B, 2015, 92, .	1.1	117
41	Efficient Promotion of Anatase TiO2 Photocatalysis via Bifunctional Surface-Terminating Tiâ^'Oâ^'Bâ^'N Structures. Journal of Physical Chemistry C, 2009, 113, 12317-12324.	1.5	115
42	Templateâ€Directed Rapid Synthesis of Pdâ€Based Ultrathin Porous Intermetallic Nanosheets for Efficient Oxygen Reduction. Angewandte Chemie - International Edition, 2021, 60, 10942-10949.	7.2	115
43	The Role of Ti as a Catalyst for the Dissociation of Hydrogen on a Mg(0001) Surface. Journal of Physical Chemistry B, 2005, 109, 18037-18041.	1.2	113
44	Implanting Ni-O-VOx sites into Cu-doped Ni for low-overpotential alkaline hydrogen evolution. Nature Communications, 2020, 11, 2720.	5.8	113
45	Sulfur doped anatase TiO2 single crystals with a high percentage of {0 0 1} facets. Journal of Colloid and Interface Science, 2010, 349, 477-483.	5.0	112
46	Extraordinary water adsorption characteristics of graphene oxide. Chemical Science, 2018, 9, 5106-5111.	3.7	112
47	Controllable CO2 electrocatalytic reduction via ferroelectric switching on single atom anchored In2Se3 monolayer. Nature Communications, 2021, 12, 5128.	5.8	110
48	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, 1682-1683.	6.6	106
49	Anisotropic Ripple Deformation in Phosphorene. Journal of Physical Chemistry Letters, 2015, 6, 1509-1513.	2.1	106
50	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, 10201-10204.	6.6	105
51	Phosphine vapor-assisted construction of heterostructured Ni₂P/NiTe₂ catalysts for efficient hydrogen evolution. Energy and Environmental Science, 2020, 13, 1799-1807.	15.6	105
52	New Family of Quantum Spin Hall Insulators in Two-dimensional Transition-Metal Halide with Large Nontrivial Band Gaps. Nano Letters, 2015, 15, 7867-7872.	4.5	104
53	The isotopic effects of deuteration on optoelectronic properties of conducting polymers. Nature Communications, 2014, 5, 3180.	5.8	103
54	Sulfurâ€Dopantâ€Promoted Electroreduction of CO₂ over Coordinatively Unsaturated Niâ€N₂ Moieties. Angewandte Chemie - International Edition, 2021, 60, 23342-23348.	7.2	98

#	Article	IF	Citations
55	Modulating Pt-O-Pt atomic clusters with isolated cobalt atoms for enhanced hydrogen evolution catalysis. Nature Communications, 2022, 13, 2430.	5.8	98
56	Surface Reconstruction of Ultrathin Palladium Nanosheets during Electrocatalytic CO₂ Reduction. Angewandte Chemie - International Edition, 2020, 59, 21493-21498.	7.2	97
57	Formation and Migration of Oxygen Vacancies in SrCoO₃ and Their Effect on Oxygen Evolution Reactions. ACS Catalysis, 2016, 6, 5565-5570.	5.5	96
58	The calculation of vibrational eigenstates by MINRES filter diagonalization. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1997, 101, 400-406.	0.9	95
59	Mg-Based Nanocomposites with High Capacity and Fast Kinetics for Hydrogen Storage. Journal of Physical Chemistry B, 2006, 110, 11697-11703.	1.2	95
60	Modelling carbon membranes for gas and isotope separation. Physical Chemistry Chemical Physics, 2013, 15, 4832.	1.3	95
61	Processable Surface Modification of Nickelâ€Heteroatom (N, S) Bridge Sites for Promoted Alkaline Hydrogen Evolution. Angewandte Chemie - International Edition, 2019, 58, 461-466.	7.2	95
62	Hydrogen Incorporation and Storage in Well-Defined Nanocrystals of Anatase Titanium Dioxide. Journal of Physical Chemistry C, 2011, 115, 25590-25594.	1.5	93
63	Photocatalytic Hydrogen Production from Water Using N-Doped Ba₅Ta₄O₁₅ under Solar Irradiation. Journal of Physical Chemistry C, 2011, 115, 15674-15678.	1.5	88
64	First principle studies of zigzag AlN nanoribbon. Chemical Physics Letters, 2009, 469, 183-185.	1.2	86
65	State-to-state reactive differential cross sections for the H+H2â†'H2+H reaction on five different potential energy surfaces employing a new quantum wavepacket computer code: DIFFREALWAVE. Journal of Chemical Physics, 2006, 125, 164303.	1.2	85
66	Borophene as a Promising Material for Charge-Modulated Switchable CO₂ Capture. ACS Applied Materials & Interfaces, 2017, 9, 19825-19830.	4.0	83
67	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.	1.7	81
68	Asymmetrically Decorated, Doped Porous Graphene As an Effective Membrane for Hydrogen Isotope Separation. Journal of Physical Chemistry C, 2012, 116, 6672-6676.	1.5	81
69	Radiationless Decay of Red Fluorescent Protein Chromophore Models via Twisted Intramolecular Charge-Transfer States. Journal of the American Chemical Society, 2007, 129, 2054-2065.	6.6	80
70	A density functional theory study on CO2 capture and activation by graphene-like boron nitride with boron vacancy. Catalysis Today, 2011, 175, 271-275.	2.2	80
71	N,P co-coordinated Fe species embedded in carbon hollow spheres for oxygen electrocatalysis. Journal of Materials Chemistry A, 2019, 7, 14732-14742.	5.2	80
72	Angular momentum conservation in unimolecular and recombination reactions. International Journal of Chemical Kinetics, 1988, 20, 307-329.	1.0	79

#	Article	IF	Citations
73	The 2.1Ã… Crystal Structure of the Far-red Fluorescent Protein HcRed: Inherent Conformational Flexibility of the Chromophore. Journal of Molecular Biology, 2005, 349, 223-237.	2.0	79
74	The effect of pH on PAMAM dendrimerâ€“siRNA complexation â€" Endosomal considerations as determined by molecular dynamics simulation. Biophysical Chemistry, 2011, 158, 126-133.	1.5	77
75	On the mechanism of gas adsorption for pristine, defective and functionalized graphene. Physical Chemistry Chemical Physics, 2017, 19, 6051-6056.	1.3	73
76	Tungsten Oxide/Carbide Surface Heterojunction Catalyst with High Hydrogen Evolution Activity. ACS Energy Letters, 2020, 5, 3560-3568.	8.8	70
77	Interfacing BiVO 4 with Reduced Graphene Oxide for Enhanced Photoactivity: A Tale of Facet Dependence of Electron Shuttling. Small, 2016, 12, 5295-5302.	5.2	68
78	Ab initio studies of hydrogen desorption from low index magnesium hydride surface. Surface Science, 2006, 600, 1854-1859.	0.8	67
79	H₂ purification by functionalized graphdiyne â€“ role of nitrogen doping. Journal of Materials Chemistry A, 2015, 3, 6767-6771.	5.2	67
80	Superâ€Exchange Interaction Induced Overall Optimization in Ferromagnetic Perovskite Oxides Enables Ultrafast Water Oxidation. Small, 2019, 15, e1903120.	5.2	67
81	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.	6.7	66
82	The controlled disassembly of mesostructured perovskites as an avenue to fabricating high performance nanohybrid catalysts. Nature Communications, 2017, 8, 15553.	5.8	65
83	Isolated Diatomic Niâ€Fe Metalâ€“Nitrogen Sites for Synergistic Electroreduction of CO₂. Angewandte Chemie, 2019, 131, 7046-7050.	1.6	65
84	The relationship between recombination, chemical activation and unimolecular dissociation rate coefficients. Journal of Chemical Physics, 1989, 90, 4265-4273.	1.2	64
85	A density functional theory study of CO2 and N2 adsorption on aluminium nitride single walled nanotubes. Journal of Materials Chemistry, 2010, 20, 10426.	6.7	62
86	Electrocatalytically Switchable CO₂ Capture: First Principle Computational Exploration of Carbon Nanotubes with Pyridinic Nitrogen. ChemSusChem, 2014, 7, 435-441.	3.6	62
87	p-Doped Graphene/Graphitic Carbon Nitride Hybrid Electrocatalysts: Unraveling Charge Transfer Mechanisms for Enhanced Hydrogen Evolution Reaction Performance. ACS Catalysis, 2016, 6, 7071-7077.	5.5	62
88	First-Principle Studies of the Formation and Diffusion of Hydrogen Vacancies in Magnesium Hydride. Journal of Physical Chemistry C, 2007, 111, 8360-8365.	1.5	61
89	Statistical modeling of ionâ€“molecule electrostatic capture. Journal of Chemical Physics, 1992, 97, 5451-5464.	1.2	60
90	Conductive Graphitic Carbon Nitride as an Ideal Material for Electrocatalytically Switchable CO2 Capture. Scientific Reports, 2015, 5, 17636.	1.6	60

#	Article	IF	Citations
91	Nitrogen doping in ion-exchangeable layered tantalate towards visible-light induced water oxidation. Chemical Communications, 2011, 47, 6293.	2.2	59
92	The origin of low workfunctions in OH terminated MXenes. Nanoscale, 2017, 9, 7016-7020.	2.8	59
93	On the microscopic mechanism of carbon gasification: A theoretical study. Carbon, 2004, 42, 2921-2928.	5.4	58
94	Boosting oxygen evolution reaction by activation of latticeâ€oxygen sites in layered Ruddlesdenâ€Popper oxide. EcoMat, 2020, 2, e12021.	6.8	58
95	Just add sugar forÂcarbohydrate induced self-assembly of curcumin. Nature Communications, 2019, 10, 582.	5.8	57
96	Electronic Regulation of Nickel Single Atoms by Confined Nickel Nanoparticles for Energyâ€Efficient CO₂ Electroreduction. Angewandte Chemie - International Edition, 2022, 61, .	7.2	57
97	A convenient procedure for the synthesis of bis-steroidal pyrazines: models for the cephalostatins. Journal of Organic Chemistry, 1992, 57, 6379-6380.	1.7	56
98	Electronic Functionality in Graphene-Based Nanoarchitectures: Discovery and Design via First-Principles Modeling. Journal of Physical Chemistry Letters, 2011, 2, 73-80.	2.1	56
99	Van der Waals-corrected density functional theory: benchmarking for hydrogenâ€“nanotube and nanotubeâ€“nanotube interactions. Nanotechnology, 2005, 16, 2118-2123.	1.3	55
100	Catalytic Effects of Subsurface Carbon in the Chemisorption of Hydrogen on a Mg(0001) Surface:Â an Ab-initio Study. Journal of Physical Chemistry B, 2006, 110, 1814-1819.	1.2	55
101	Confinement of Ionic Liquids at Single-Ni-Sites Boost Electroreduction of CO₂ in Aqueous Electrolytes. ACS Catalysis, 2020, 10, 13171-13178.	5.5	54
102	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.	1.5	53
103	An Ultra-Long-Life Flexible Lithiumâ€“Sulfur Battery with Lithium Cloth Anode and Polysulfone-Functionalized Separator. ACS Nano, 2021, 15, 1358-1369.	7.3	53
104	Full Iterative Solution of the Two-Dimensional Master Equation for Thermal Unimolecular Reactions. The Journal of Physical Chemistry, 1996, 100, 7090-7096.	2.9	52
105	First-Principle Study of Adsorption of Hydrogen on Ti-Doped Mg(0001) Surface. Journal of Physical Chemistry B, 2006, 110, 21747-21750.	1.2	52
106	Conductive Boron-Doped Graphene as an Ideal Material for Electrocatalytically Switchable and High-Capacity Hydrogen Storage. ACS Applied Materials & Interfaces, 2016, 8, 32815-32822.	4.0	52
107	Convergent Proton-Transfer Photocycles Violate Mirror-Image Symmetry in a Key Melanin Monomer. Journal of the American Chemical Society, 2007, 129, 6672-6673.	6.6	51
108	Understanding the high activity of mildly reduced graphene oxide electrocatalysts in oxygen reduction to hydrogen peroxide. Materials Horizons, 2019, 6, 1409-1415.	6.4	51

#	Article	IF	Citations
109	Comparative study of hydrogen storage in Li- and K-doped carbon materialsâ€“â€“theoretically revisited. Carbon, 2004, 42, 2509-2514.	5.4	50
110	Strong Interaction between Gold and Anatase TiO₂(001) Predicted by First Principle Studies. Journal of Physical Chemistry C, 2012, 116, 3524-3531.	1.5	50
111	Pyrite-type ruthenium disulfide with tunable disorder and defects enables ultra-efficient overall water splitting. Journal of Materials Chemistry A, 2019, 7, 14222-14232.	5.2	50
112	Regulating electron transfer over asymmetric low-spin Co(II) for highly selective electrocatalysis. Chem Catalysis, 2022, 2, 372-385.	2.9	50
113	Mobile Polaronic States in Î±-MoO₃: An ab Initio Investigation of the Role of Oxygen Vacancies and Alkali Ions. ACS Applied Materials & Interfaces, 2016, 8, 10911-10917.	4.0	49
114	Numerical study of hydrogenic effective mass theory for an impurity P donor in Si in the presence of an electric field and interfaces. Physical Review B, 2003, 68, .	1.1	48
115	The dynamics of the H⁺+ D₂reaction: a comparison of quantum mechanical wavepacket, quasi-classical and statistical-quasi-classical results. Physical Chemistry Chemical Physics, 2010, 12, 1102-1115.	1.3	48
116	Theoretical Predictions of Freestanding Honeycomb Sheets of Cadmium Chalcogenides. Journal of Physical Chemistry C, 2014, 118, 16236-16245.	1.5	48
117	Structure, Dynamics, and Energetics of siRNAâˆ’Cationic Vector Complexation: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2010, 114, 9220-9230.	1.2	47
118	Stacking-Dependent Interlayer Magnetic Coupling in 2D CrI₃/CrGeTe₃ Nanostructures for Spintronics. ACS Applied Nano Materials, 2020, 3, 1282-1288.	2.4	47
119	Angularâ€momentum resolution in transitionalâ€mode state counting for loose transition states. Journal of Chemical Physics, 1992, 97, 2406-2416.	1.2	46
120	Lattice Distortion Oriented Angular Self-Assembly of Monolayer Titania Sheets. Journal of the American Chemical Society, 2011, 133, 695-697.	6.6	46
121	Role of charge in destabilizingAlH4andBH4complex anions for hydrogen storage applications:Ab initiodensity functional calculations. Physical Review B, 2006, 74, .	1.1	45
122	Diluted Magnetic Semiconductor Nanowires Prepared by the Solutionâ€“Liquidâ€“Solid Method. Angewandte Chemie - International Edition, 2010, 49, 2777-2781.	7.2	45
123	Antipoisoning Nickelâ€“Carbon Electrocatalyst for Practical Electrochemical CO₂ Reduction to CO. ACS Applied Energy Materials, 2019, 2, 8002-8009.	2.5	45
124	Entropy barriers to proton transfer. Journal of the American Chemical Society, 1991, 113, 862-869.	6.6	44
125	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.	3.0	43
126	Structure and Dynamics of Multiple Cationic Vectorsâˆ’siRNA Complexation by All-Atomic Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 9231-9237.	1.2	43

#	Article	IF	Citations
127	Layered Grapheneâ€“Hexagonal BN Nanocomposites: Experimentally Feasible Approach to Chargeâ€Induced Switchable CO₂ Capture. ChemSusChem, 2015, 8, 2987-2993.	3.6	43
128	Ab initio modelling of basal plane oxidation of graphenes and implications for modelling char combustion. Carbon, 2002, 40, 2341-2349.	5.4	42
129	Calculation of quantum resonance energies and lifetimes via quasi-minimum residual filter diagonalization. Chemical Physics Letters, 1998, 283, 69-76.	1.2	41
130	Lanczos subspace filter diagonalization: Homogeneous recursive filtering and a low-storage method for the calculation of matrix elements. Physical Chemistry Chemical Physics, 2001, 3, 2282-2288.	1.3	41
131	Kinetic isotope effect for ground state proton transfer in the green fluorescent protein: a quantum-kinetic model. Physical Chemistry Chemical Physics, 2009, 11, 8422.	1.3	41
132	Light-Induced Synergistic Multidefect Sites on TiO₂/SiO₂ Composites for Catalytic Dehydrogenation. ACS Catalysis, 2019, 9, 2674-2684.	5.5	41
133	Intercalation of Sulfonate into Layered Double Hydroxide: Comparison of Simulation with Experiment. Journal of Physical Chemistry C, 2009, 113, 559-566.	1.5	40
134	Autocatalytic Surface Reductionâ€Assisted Synthesis of PtW Ultrathin Alloy Nanowires for Highly Efficient Hydrogen Evolution Reaction. Advanced Energy Materials, 2022, 12, .	10.2	40
135	A master equation model for bimolecular reaction via multi-well isomerizing intermediates. Physical Chemistry Chemical Physics, 2000, 2, 793-803.	1.3	38
136	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.	1.9	37
137	A formation mechanism of oxygen vacancies in a MnO2 monolayer: a DFT + U study. Physical Chemistry Chemical Physics, 2011, 13, 11325.	1.3	37
138	Charge Modulation in Graphitic Carbon Nitride as a Switchable Approach to Highâ€Capacity Hydrogen Storage. ChemSusChem, 2015, 8, 3626-3631.	3.6	37
139	Surface Reconstruction of Ultrathin Palladium Nanosheets during Electrocatalytic CO₂ Reduction. Angewandte Chemie, 2020, 132, 21677-21682.	1.6	37
140	Microscopic rate coefficients in reactions with flexible transition states: Analysis of the transitionalâ€mode sum of states. Journal of Chemical Physics, 1991, 95, 3404-3430.	1.2	36
141	Integral and differential cross sections for the S(1D)+HD reaction employing the ground adiabatic electronic state. Physical Chemistry Chemical Physics, 2009, 11, 11587.	1.3	36
142	Modulation Doping of Silicon using Aluminium-induced Acceptor States in Silicon Dioxide. Scientific Reports, 2017, 7, 46703.	1.6	36
143	Efficient Water Splitting Actualized through an Electrochemistryâ€Induced Heteroâ€Structured Antiperovskite/(Oxy)Hydroxide Hybrid. Small, 2020, 16, e2006800.	5.2	36
144	Angular momentum conservation in multichannel unimolecular reactions. International Journal of Chemical Kinetics, 1988, 20, 979-990.	1.0	35

#	Article	IF	Citations
145	MODEL REAL-TIME QUANTUM DYNAMICAL SIMULATIONS OF PROTON TRANSFER IN THE GREEN FLUORESCENT PROTEIN (GFP). Journal of Theoretical and Computational Chemistry, 2007, 06, 789-802.	1.8	35
146	Synthesis and Characterization of Colloidal Coreâ€“Shell Semiconductor Nanowires. European Journal of Inorganic Chemistry, 2010, 2010, 4325-4331.	1.0	35
147	The Role of Atomic Vacancy on Water Dissociation over Titanium Dioxide Nanosheet: A Density Functional Theory Study. Journal of Physical Chemistry C, 2012, 116, 2477-2482.	1.5	35
148	Exceptional Optoelectronic Properties of Hydrogenated Bilayer Silicene. Physical Review X, 2014, 4, .	2.8	35
149	Tetragonal bismuth bilayer: a stable and robust quantum spin hall insulator. 2D Materials, 2015, 2, 045010.	2.0	34
150	Versatile electrocatalytic processes realized by Ni, Co and Fe alloyed core coordinated carbon shells. Journal of Materials Chemistry A, 2019, 7, 12154-12165.	5.2	34
151	Rapid algorithms for microcanonical variational Rice-Ramsperger-Kassel-Marcus theory. The Journal of Physical Chemistry, 1993, 97, 7034-7039.	2.9	33
152	Calculation of product state distributions from resonance decay via Lanczos subspace filter diagonalization: Application to HO2. Journal of Chemical Physics, 2001, 115, 5751-5758.	1.2	33
153	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.	1.2	33
154	Electrocatalytic Reduction of Carbon Dioxide to Methane on Single Transition Metal Atoms Supported on a Defective Boron Nitride Monolayer: First Principle Study. Advanced Theory and Simulations, 2019, 2, 1800094.	1.3	33
155	The pressure dependence of ionâ€“molecule association rate coefficients. Journal of Chemical Physics, 1989, 90, 1630-1640.	1.2	32
156	OH-Initiated Oxidation of Toluene. 1. Quantum Chemistry Investigation of the Reaction Pathâ€. Journal of Physical Chemistry A, 2007, 111, 3686-3690.	1.1	32
157	Study of the H+O2 reaction by means of quantum mechanical and statistical approaches: The dynamics on two different potential energy surfaces. Journal of Chemical Physics, 2008, 128, 244308.	1.2	32
158	Unraveling Photocatalytic Mechanism and Selectivity in PETâ€RAFT Polymerization. Advanced Theory and Simulations, 2019, 2, 1900038.	1.3	32
159	Tailored Brownmillerite Oxide Catalyst with Multiple Electronic Functionalities Enables Ultrafast Water Oxidation. Chemistry of Materials, 2021, 33, 5233-5241.	3.2	32
160	Variational transition state theory: a simple model for dissociation and recombination reactions of small species. The Journal of Physical Chemistry, 1991, 95, 8685-8694.	2.9	31
161	Application of inverse iteration to 2-dimensional master equations. Journal of Computational Chemistry, 1997, 18, 1004-1010.	1.5	31
162	Half metallicty in finite-length zigzag single walled carbon nanotube: A first-principle prediction. Applied Physics Letters, 2008, 93, 073101.	1.5	31

#	Article	IF	Citations
163	Encapsulated Silicene: A Robust Large-Gap Topological Insulator. ACS Applied Materials & Interfaces, 2015, 7, 19226-19233.	4.0	31
164	Sc and Nb dopants in SrCoO3 modulate electronic and vacancy structures for improved water splitting and SOFC cathodes. Energy Storage Materials, 2017, 9, 229-234.	9.5	31
165	Theoretical investigation of the potential energy surface for the NH2+NO reaction via density functional theory and ab initio molecular electronic structure theory. Journal of Chemical Physics, 1997, 106, 9236-9251.	1.2	30
166	State-to-state reaction probabilities for the H+O2(v,j)â†'O+OH(vâ€²,jâ€²) reaction on three potential energy surfaces. Journal of Chemical Physics, 2007, 127, 064316.	1.2	29
167	The catalytic role of an isolated-Ti atom in the hydrogenation of Ti-doped Al(001) surface: An ab initio density functional theory calculation. Chemical Physics Letters, 2007, 450, 80-85.	1.2	29
168	Exact and truncated Coriolis coupling calculations for the S(1D)+HD reaction employing the ground adiabatic electronic state. Physical Chemistry Chemical Physics, 2010, 12, 12711.	1.3	29
169	Kinetic modelling of molecular hydrogen transport in microporous carbon materials. Physical Chemistry Chemical Physics, 2011, 13, 7834.	1.3	29
170	A Structural Basis for the pH-dependent Increase in Fluorescence Efficiency of Chromoproteins. Journal of Molecular Biology, 2007, 368, 998-1010.	2.0	28
171	QM/MM studies of structural and energetic properties of the far-red fluorescent protein HcRed. Physical Chemistry Chemical Physics, 2010, 12, 2450.	1.3	28
172	Bandgap narrowing of titanium oxide nanosheets: homogeneous doping of molecular iodine for improved photoreactivity. Journal of Materials Chemistry, 2011, 21, 14672.	6.7	28
173	Multiple Hydrogen-Bonded Complexes Based on 2-Ureido-4[1H]-pyrimidinone: A Theoretical Study. Journal of Physical Chemistry B, 2011, 115, 11053-11062.	1.2	28
174	Production and loss of HC3N in interstellar clouds: some relevant laboratory measurements. Monthly Notices of the Royal Astronomical Society, 1986, 219, 89-94.	1.6	27
175	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.	2.9	27
176	The role of V2O5 on the dehydrogenation and hydrogenation in magnesium hydride: An ab initio study. Applied Physics Letters, 2008, 92, .	1.5	27
177	Anatomy of the S(1D) + H2 reaction: the dynamics on two new potential energy surfaces from quantum dynamics calculations. Physical Chemistry Chemical Physics, 2011, 13, 13645.	1.3	26
178	Structures, Energetics, and Electronic Properties of Layered Materials and Nanotubes of Cadmium Chalcogenides. Journal of Physical Chemistry C, 2013, 117, 25817-25825.	1.5	26
179	Charge-controlled switchable H2 storage on conductive borophene nanosheet. International Journal of Hydrogen Energy, 2019, 44, 20150-20157.	3.8	26
180	Multiple-Well Isomerization Diffusion Equation Solutions with a Shift and Invert Lanczos Algorithm. Journal of Physical Chemistry A, 1997, 101, 5765-5769.	1.1	25

#	Article	IF	Citations
181	Mechanistic aspects of proton chain transfer in the green fluorescent protein : Part II. A comparison of minimal quantum chemical models. Physical Chemistry Chemical Physics, 2007, 9, 452-458.	1.3	25
182	High-performance polymer photovoltaics based on rationally designed fullerene acceptors. Solar Energy Materials and Solar Cells, 2013, 118, 171-178.	3.0	25
183	Hexagonal boron nitride and graphene in-plane heterostructures: An experimentally feasible approach to charge-induced switchable CO 2 capture. Chemical Physics, 2016, 478, 139-144.	0.9	25
184	Computational design of two-dimensional nanomaterials for charge modulated CO2/H2 capture and/or storage. Energy Storage Materials, 2017, 8, 169-183.	9.5	25
185	Kinetics and Product Branching Ratios for the Reaction HCO + NO2. The Journal of Physical Chemistry, 1995, 99, 7473-7481.	2.9	24
186	The simulation of outgoing-wave boundary conditions via a symmetrically damped, Hermitian Hamiltonian operator. Journal of Chemical Physics, 1997, 107, 9985-9993.	1.2	24
187	The Elimination of Lanczos Ghosting Effects by MINRES Filter Diagonalization. Journal of Computational Physics, 1998, 143, 484-494.	1.9	24
188	Classical flux integrals in transition state theory: Generalized reaction coordinates. Journal of Chemical Physics, 1999, 111, 1830-1842.	1.2	24
189	Chebyshev real wave packet propagation: H+O2 (J=0) state-to-state reactive scattering calculations. Journal of Chemical Physics, 2002, 117, 5174-5182.	1.2	24
190	Converged quantum calculations of HO2 bound states and resonances for J=6 and 10. Journal of Chemical Physics, 2004, 120, 9583-9593.	1.2	24
191	Mechanistic Aspects of Proton Chain Transfer:Â A Computational Study for the Green Fluorescent Protein Chromophore. Journal of Physical Chemistry B, 2006, 110, 5084-5093.	1.2	24
192	Formation of Single-Walled Carbon Nanotube via the Interaction of Graphene Nanoribbons:â€‰ Ab Initio Density Functional Calculations. Nano Letters, 2007, 7, 3349-3354.	4.5	24
193	Oxygen vacancy induced structural variations of exfoliated monolayerMnO2sheets. Physical Review B, 2010, 81, .	1.1	24
194	Theoretical study of two states reactivity of methane activation on iron atom and iron dimer. Fuel, 2012, 96, 291-297.	3.4	24
195	Growth and Electrochemical Characterization of Carbon Nanospike Thin Film Electrodes. Journal of the Electrochemical Society, 2014, 161, H558-H563.	1.3	24
196	Charge-modulated permeability and selectivity in graphdiyne for hydrogen purification. Molecular Simulation, 2016, 42, 573-579.	0.9	24
197	Time-dependent master equation simulation of complex elementary reactions in combustion: Application to the reaction of 1CH2 with C2H2 from 300Ã¢â‚¬â€œ2000 K. Faraday Discussions, 2001, 119, 159-171.	1.6	23
198	Calculation of bound and resonance states of HO2 for nonzero total angular momentum. Journal of Chemical Physics, 2003, 118, 10042-10050.	1.2	23

#	Article	IF	Citations
199	Non-equilibrium dynamics, materials and structures for hot carrier solar cells: a detailed review. Semiconductor Science and Technology, 2020, 35, 073002.	1.0	23
200	The effect of Fe doping on adsorption of CO₂/N₂within carbon nanotubes: a density functional theory study with dispersion corrections. Nanotechnology, 2009, 20, 375701.	1.3	22
201	Charge carrier exchange at chemically modified graphene edges: a density functional theory study. Journal of Materials Chemistry, 2012, 22, 8321.	6.7	22
202	How to achieve maximum charge carrier loading on heteroatom-substituted graphene nanoribbon edges: density functional theory study. Journal of Materials Chemistry, 2012, 22, 13751.	6.7	22
203	Chemically modified ribbon edge stimulated H2 dissociation: a first-principles computational study. Physical Chemistry Chemical Physics, 2013, 15, 8054.	1.3	22
204	Defect Engineering in Graphene-Confined Single-Atom Iron Catalysts for Room-Temperature Methane Conversion. Journal of Physical Chemistry C, 2021, 125, 12628-12635.	1.5	22
205	Microscopic reaction rates in ion/molecule reactions: effects of uncoupled modes. The Journal of Physical Chemistry, 1989, 93, 8142-8148.	2.9	21
206	Quantum dynamical study of the O(D1)+HCl reaction employing three electronic state potential energy surfaces. Journal of Chemical Physics, 2008, 128, 014308.	1.2	21
207	Interaction of Water with the Fluorine-Covered Anatase TiO₂ (001) Surface. Journal of Physical Chemistry C, 2011, 115, 17092-17096.	1.5	21
208	Structured water in polyelectrolyte dendrimers: Understanding small angle neutron scattering results through atomistic simulation. Journal of Chemical Physics, 2012, 136, 144901.	1.2	21
209	Understanding the Charge Transfer at the Interface of Electron Donors and Acceptors: TTFâ€“TCNQ as an Example. ACS Applied Materials & Interfaces, 2017, 9, 27266-27272.	4.0	21
210	Statistical modeling of capture, association, and exitâ€channel dynamics in the CH3+/CH3CN system. Journal of Chemical Physics, 1993, 98, 1944-1956.	1.2	20
211	Removal of Orthodontic Bonding Resin Residues by CO₂Laser Radiation: Surface Effects. Photomedicine and Laser Surgery, 1999, 17, 13-18.	1.1	20
212	Isomerization mechanism of the HcRed fluorescent protein chromophore. Physical Chemistry Chemical Physics, 2012, 14, 11413.	1.3	20
213	Materials design for electrocatalytic carbon capture. APL Materials, 2016, 4, .	2.2	20
214	Dynamical Interactions of 5-Fluorouracil Drug with Dendritic Peptide Vectors: The Impact of Dendrimer Generation, Charge, Counterions, and Structured Water. Journal of Physical Chemistry B, 2016, 120, 5732-5743.	1.2	20
215	Light, Catalyst, Activation: Boosting Catalytic Oxygen Activation Using a Light Pretreatment Approach. ACS Catalysis, 2017, 7, 3644-3653.	5.5	20
216	A molecular-level strategy to boost the mass transport of perovskite electrocatalyst for enhanced oxygen evolution. Applied Physics Reviews, 2021, 8, .	5.5	20

#	Article	IF	Citations
217	Theoretical Studies of Chromophore Maturation in the Wild-Type Green Fluorescent Protein: ONIOM(DFT:MM) Investigation of the Mechanism of Cyclization. Journal of Physical Chemistry B, 2012, 116, 1426-1436.	1.2	19
218	Processable Surface Modification of Nickelâ€Heteroatom (N, S) Bridge Sites for Promoted Alkaline Hydrogen Evolution. Angewandte Chemie, 2018, 131, 471.	1.6	19
219	Theoretical Study of the Reaction CH(Î§2Î) + NO(Î§2Î). 3. Determination of the Branching Ratios. Journal of Physical Chemistry A, 1998, 102, 3358-3367.	1.1	18
220	Methane activation on Fe4 cluster: A density functional theory study. Chemical Physics Letters, 2012, 550, 41-46.	1.2	18
221	Density functional theory study on adsorption of Pt nanoparticle on graphene. International Journal of Hydrogen Energy, 2013, 38, 6283-6287.	3.8	18
222	First-Principle Framework for Total Charging Energies in Electrocatalytic Materials and Charge-Responsive Molecular Binding at Gasâ€“Surface Interfaces. ACS Applied Materials & Interfaces, 2016, 8, 10897-10903.	4.0	18
223	Restarted Krylov-space spectral filtering. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 861-869.	1.7	17
224	Subspace wavepacket evolution with Newton polynomials. Chemical Physics Letters, 2001, 336, 149-155.	1.2	17
225	Addition of diazomethane to armchair single-walled carbon nanotubes and their reaction sequences: A computational study. Chemical Physics Letters, 2007, 436, 218-223.	1.2	17
226	Computer Modeling Study for Intercalation of Drug Heparin into Layered Double Hydroxide. Journal of Physical Chemistry C, 2010, 114, 12618-12629.	1.5	17
227	Optimal spectral filtering in a finite subspace: a Lanczos-based implementation. Physical Chemistry Chemical Physics, 1999, 1, 1311-1316.	1.3	16
228	Lanczos Subspace Time-Independent Wave Packet Calculations of S (1D) + H2Reactive Scattering. Journal of Physical Chemistry A, 2002, 106, 6137-6142.	1.1	16
229	HO2 Ro-Vibrational Bound-State Calculations for Large Angular Momentum: J = 30, 40, and 50. Journal of Physical Chemistry A, 2006, 110, 3246-3253.	1.1	16
230	Determination of chromophore charge states in the low pH color transition of the fluorescent protein Rtms5H146S via time-dependent DFT. Chemical Physics Letters, 2006, 420, 507-511.	1.2	16
231	Molecular orbital calculations of two-electron states for P-donor solid-state spin qubits. Physical Review B, 2006, 73, .	1.1	16
232	Orbital engineering of two-dimensional materials with hydrogenation: A realization of giant gap and strongly correlated topological insulators. Physical Review B, 2015, 92, .	1.1	16
233	Peculiarity of Two Thermodynamically-Stable Morphologies and Their Impact on the Efficiency of Small Molecule Bulk Heterojunction Solar Cells. Scientific Reports, 2015, 5, 13407.	1.6	16
234	Cooperative defect-enriched SiO2 for oxygen activation and organic dehydrogenation. Journal of Catalysis, 2019, 376, 168-179.	3.1	16

#	Article	IF	Citations
235	Flux Factors in Variational Transition-State Theory. The Journal of Physical Chemistry, 1994, 98, 6496-6504.	2.9	15
236	On the calculation of absolute spectral densities. Journal of Chemical Physics, 1996, 105, 4055-4064.	1.2	15
237	A comparison of low-storage strategies for spectral analysis in dissipative systems: filter diagonalisation in the Lanczos representation and harmonic inversion of the Chebychev-order-domain autocorrelation function. Chemical Physics Letters, 2001, 347, 211-219.	1.2	15
238	Effect of Dimerization on Vibrational Spectra of Eumelanin Precursors^{â€}. Photochemistry and Photobiology, 2008, 84, 613-619.	1.3	15
239	Numerical solution methods for large, difficult kinetic master equations. Theoretical Chemistry Accounts, 2009, 124, 303-317.	0.5	15
240	The Mechanism of Cyclization in Chromophore Maturation of Green Fluorescent Protein: A Theoretical Study. Journal of Physical Chemistry B, 2010, 114, 9698-9705.	1.2	15
241	Cobalt-doped cadmium selenide colloidal nanowires. Chemical Communications, 2011, 47, 11894.	2.2	15
242	Controlling molecular ordering in solution-state conjugated polymers. Nanoscale, 2015, 7, 15134-15141.	2.8	15
243	Binding and Release between Polymeric Carrier and Protein Drug: pH-Mediated Interplay of Coulomb Forces, Hydrogen Bonding, van der Waals Interactions, and Entropy. Biomacromolecules, 2017, 18, 3665-3677.	2.6	15
244	Intrinsic ultrasmall nanoscale silicon turns n-/p-type with SiO₂/Si₃N₄-coating. Beilstein Journal of Nanotechnology, 2018, 9, 2255-2264.	1.5	15
245	Facet-dependent carrier dynamics of cuprous oxide regulating the photocatalytic hydrogen generation. Materials Advances, 2022, 3, 2200-2212.	2.6	15
246	Towards quantum mechanical characterization of the dissociation dynamics of ketene. Faraday Discussions, 1995, 102, 17.	1.6	14
247	Time evolution in the unimolecular master equation at low temperatures: full spectral solution with scalable iterative methods and high precision. Computer Physics Communications, 2001, 141, 39-54.	3.0	14
248	Quantum Mechanical Calculation of Energy Dependence of OCl/OH Product Branching Ratio and Product Quantum State Distributions for the O(¹D) + HCl Reaction on All Three Contributing Electronic State Potential Energy Surfaces. Journal of Physical Chemistry A, 2008, 112, 7947-7960.	1.1	14
249	Molecular Modeling of Hydrotalcite Structure Intercalated with Transition Metal Oxide Anions: CrO42â€“and VO43â€“. Journal of Physical Chemistry A, 2011, 115, 13673-13683.	1.1	14
250	Quantum calculations for the S(1D)+H2reaction employing the ground adiabatic electronic state. Physica Scripta, 2011, 84, 028102.	1.2	14
251	High-mobility anisotropic transport in few-layer Î³-B₂₈films. Nanoscale, 2016, 8, 20111-20117.	2.8	14
252	Calculation of the vibrational spectral density of NO2 via density correlation functions. Chemical Physics Letters, 1997, 273, 55-61.	1.2	13

#	Article	IF	Citations
253	Unimolecular rovibrational bound and resonance states for large angular momentum: J=20 calculations for HO2. Journal of Chemical Physics, 2005, 123, 014308.	1.2	13
254	OH-Initiated Oxidation of Toluene. 2. Master Equation Simulation of Toluene Oxide Isomerizationâ€. Journal of Physical Chemistry A, 2007, 111, 3691-3696.	1.1	13
255	Energy dependent dynamics of the O(1D) + HCl reaction: A quantum, quasiclassical and statistical study. Physical Chemistry Chemical Physics, 2011, 13, 8502.	1.3	13
256	Synthesis, optical properties and theoretical modelling of discrete emitting states in doped silicon nanocrystals for bioimaging. Nanoscale, 2018, 10, 15600-15607.	2.8	13
257	Calculation of absolute spectral densities via stochastic estimators of tr{Î´(E - Ä)}. Chemical Physics Letters, 1997, 278, 345-351.	1.2	12
258	A pseudospectral algorithm for the computation of transitional-mode eigenfunctions in loose transition states. II. Optimized primary and grid representations. Journal of Chemical Physics, 1999, 110, 1354-1364.	1.2	12
259	Solving the unimolecular master equation with a weighted subspace projection method. Journal of Computational Chemistry, 2000, 21, 592-606.	1.5	12
260	Kinematic Factors in Transition State Theory with a Generalized Reaction Coordinateâ€. Journal of Physical Chemistry A, 2000, 104, 10489-10499.	1.1	12
261	Selecting Methods to Solve Multi-Well Master Equations. Journal of Theoretical and Computational Chemistry, 2003, 02, 179-191.	1.8	12
262	Vacancy mediated desorption of hydrogen from a sodium alanate surface: An ab initio spin-polarized study. Applied Physics Letters, 2007, 90, 143119.	1.5	12
263	Computational study of methyl derivatives of ammonia borane for hydrogen storage. Physical Chemistry Chemical Physics, 2008, 10, 6104.	1.3	12
264	Reducible Disulfide-Based Non-Viral Gene Delivery Systems. Mini-Reviews in Medicinal Chemistry, 2009, 9, 1242-1250.	1.1	12
265	Charge-Dependent Dynamics of a Polyelectrolyte Dendrimer and Its Correlation with Invasive Water. Journal of the American Chemical Society, 2013, 135, 5111-5117.	6.6	12
266	Nitrogen Doped Carbon Nanosheets Coupled Nickelâ€“Carbon Pyramid Arrays Toward Efficient Evolution of Hydrogen. Advanced Sustainable Systems, 2017, 1, 1700032.	2.7	12
267	A comparison of an experimental unimolecular lifetime distribution with Riceâ€“Ramspergerâ€“Kasselâ€“Marcus theory. Journal of Chemical Physics, 1994, 100, 5696-5705.	1.2	11
268	A pseudo-spectral algorithm for the computation of transitional-mode eigenfunctions in loose transition states. Chemical Physics Letters, 1995, 243, 359-366.	1.2	11
269	Reversibility Relationship in Collision-Complex-Forming Bimolecular Reactions. Journal of Physical Chemistry A, 1997, 101, 7311-7314.	1.1	11
270	A real symmetric Lanczos subspace implementation of quantum scattering using boundary inhomogeneities. Chemical Physics Letters, 2002, 366, 390-397.	1.2	11

#	Article	IF	Citations
271	transâ€“cis Isomerism and acylimine formation in DsRed chromophore models: Intrinsic rotation barriers. Chemical Physics Letters, 2006, 426, 159-162.	1.2	11
272	Weak competing interactions control assembly of strongly bonded TCNQ ionic acceptor molecules on silver surfaces. Physical Review B, 2014, 90, .	1.1	11
273	Unveiling the role of carbon oxidation in irreversible degradation of atomically-dispersed FeN₄ moieties for proton exchange membrane fuel cells. Journal of Materials Chemistry A, 2021, 9, 8721-8729.	5.2	11
274	Full S matrix calculation via a single real-symmetric Lanczos recursion: The Lanczos artificial boundary inhomogeneity method. Journal of Chemical Physics, 2004, 120, 1161-1163.	1.2	10
275	Iterative quantum computations of HO2 bound states and resonances for J = 4 and 5. Physical Chemistry Chemical Physics, 2004, 6, 4240.	1.3	10
276	Role of Lithium Vacancies in Accelerating the Dehydrogenation Kinetics on a LiBH₄(010) Surface:â€‰ An Ab Initio Study. Journal of Physical Chemistry C, 2007, 111, 12124-12128.	1.5	10
277	In Operando Selfâ€Healing of Perovskite Electrocatalysts: A Case Study of SrCoO₃ for the Oxygen Evolution Reaction. Particle and Particle Systems Characterization, 2017, 34, 1600280.	1.2	10
278	Electronic Structure Shift of Deeply Nanoscale Silicon by <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mi>Si</mml:mi><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math> versus <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mi>Si</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi	1.5	10
279	Theory-guided construction of electron-deficient sites via removal of lattice oxygen for the boosted electrocatalytic synthesis of ammonia. Nano Research, 2021, 14, 1457-1464.	5.8	10
280	Fast, scalable master equation solution algorithms. IV. Lanczos iteration with diffusion approximation preconditioned iterative inversion. Journal of Chemical Physics, 2003, 119, 12741-12748.	1.2	9
281	The effects of J-gate potential and interfaces on donor exchange coupling in the Kane quantum computer architecture. Journal of Physics Condensed Matter, 2004, 16, 1011-1023.	0.7	9
282	Leading coordinate analysis of reaction pathways in proton chain transfer: Application to a two-proton transfer model for the green fluorescent protein. Chemical Physics, 2006, 326, 204-209.	0.9	9
283	First Principle Study of Hydrogenation of MgB₂: An Important Step Toward Reversible Hydrogen Storage in the Coupled LiBH₄/MgH₂ System. Journal of Nanoscience and Nanotechnology, 2009, 9, 4388-4391.	0.9	9
284	First principle study of proton transfer in the green fluorescent protein (GFP): Ab initio PES in a cluster model. Computational and Theoretical Chemistry, 2012, 990, 185-193.	1.1	9
285	The mechanism of dehydration in chromophore maturation of wild-type green fluorescent protein: A theoretical study. Chemical Physics Letters, 2015, 631-632, 42-46.	1.2	9
286	The mechanism of oxidation in chromophore maturation of wild-type green fluorescent protein: a theoretical study. Physical Chemistry Chemical Physics, 2017, 19, 12942-12952.	1.3	9
287	Templateâ€Directed Rapid Synthesis of Pdâ€Based Ultrathin Porous Intermetallic Nanosheets for Efficient Oxygen Reduction. Angewandte Chemie, 2021, 133, 11037-11044.	1.6	9
288	Sulfurâ€Dopantâ€Promoted Electroreduction of CO 2 over Coordinatively Unsaturated Niâ€N 2 Moieties. Angewandte Chemie, 0, , .	1.6	9

#	Article	IF	Citations
289	Electronic Regulation of Nickel Single Atoms by Confined Nickel Nanoparticles for Energyâ€Efficient CO₂ Electroreduction. Angewandte Chemie, 2022, 134, .	1.6	9
290	Prediction of absolute rate coefficients and product branching ratios for the C(3P)+allene reaction system. Journal of Chemical Physics, 2002, 117, 7055-7067.	1.2	8
291	Calculation of Resonances and Product State Distributions for the Unimolecular Dissociation of H2S. Journal of Physical Chemistry A, 2002, 106, 6129-6136.	1.1	8
292	Fast, scalable master equation solution algorithms. III. Direct time propagation accelerated by a diffusion approximation preconditioned iterative solver. Journal of Chemical Physics, 2003, 119, 12729-12740.	1.2	8
293	The 2.0 Ã... Crystal Structure of a Pocilloporin at pH 3.5: The Structural Basis for the Linkage Between Color Transition and Halide Binding. Photochemistry and Photobiology, 2006, 82, 359.	1.3	8
294	Quantum mechanical calculations of the S(¹D)+HD reaction dynamics on the ground electronic state. Journal of Physics: Conference Series, 2009, 185, 012056.	0.3	8
295	Improved visible light absorption of HTaWO6 induced by nitrogen doping: An experimental and theoretical study. Chemical Physics Letters, 2011, 501, 427-430.	1.2	8
296	Charge-modulated CO2 capture. Current Opinion in Electrochemistry, 2017, 4, 118-123.	2.5	8
297	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mi>Si</mml:mi><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math> Modulation Doping for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Si</mml:mi></mml:math> : Acceptor Candidates. Physical Review Applied, 2018, 10, .	1.5	8
298	Application of contracted distributed approximating functions to solving vibrational eigenvalue problems. Journal of Chemical Physics, 1999, 110, 72-79.	1.2	7
299	Flexibility of Short-Strand RNA in Aqueous Solution as Revealed by Molecular Dynamics Simulation: Are A-RNA and AÂ´-RNA Distinct Conformational Structures?. Australian Journal of Chemistry, 2009, 62, 1054.	0.5	7
300	Formation energies of low-indexed surfaces of tin dioxide terminated by nonmetals. Solid State Communications, 2010, 150, 957-960.	0.9	7
301	Adsorption and Dissociation of Ammonia Borane Outside and Inside Single-Walled Carbon Nanotubes: A Density Functional Theory Study. Journal of Physical Chemistry C, 2011, 115, 12580-12585.	1.5	7
302	Hydrotalcite Intercalated siRNA: Computational Characterization of the Interlayer Environment. Pharmaceutics, 2012, 4, 296-313.	2.0	7
303	Molecular dynamics and neutron scattering study of the dependence of polyelectrolyte dendrimer conformation on counterion behavior. Journal of Chemical Physics, 2012, 137, 064902.	1.2	7
304	Oxygen Electrocatalysis at Mn^{III}â€“O_xâ€“C Hybrid Heterojunction: An Electronic Synergy or Cooperative Catalysis?. ACS Applied Materials & Interfaces, 2019, 11, 706-713.	4.0	7
305	Facile CO Oxidation on Oxygenâ€functionalized MXenes via the Marsâ€van Krevelen Mechanism. ChemCatChem, 2020, 12, 1007-1012.	1.8	7
306	Turning Low-Nanoscale Intrinsic Silicon Highly Electron-Conductive by SiO2 Coating. ACS Applied Materials & Interfaces, 2021, 13, 20479-20488.	4.0	7

#	Article	IF	Citations
307	Vanadium Oxide Clusters Decorated Metallic Cobalt Catalyst for Active Alkaline Hydrogen Evolution. Cell Reports Physical Science, 2020, 1, 100275.	2.8	7
308	A COMPARATIVE STUDY OF ITERATIVE CHEBYSHEV AND LANCZOS IMPLEMENTATIONS OF THE BOUNDARY INHOMOGENEITY METHOD FOR QUANTUM SCATTERING. Journal of Theoretical and Computational Chemistry, 2003, 02, 563-571.	1.8	6
309	HOCl Ro-Vibrational Bound-State Calculations for Nonzero Total Angular Momentumâ€. Journal of Physical Chemistry A, 2006, 110, 5468-5474.	1.1	6
310	Quantum Calculation of Ro-vibrational States:â€‰ Methodology and DOCl Application Results. Journal of Physical Chemistry A, 2008, 112, 4141-4147.	1.1	6
311	Structural and Relaxation Effects in Proton Wire Energetics: Model Studies of the Green Fluorescent Protein Photocycle. Australian Journal of Chemistry, 2010, 63, 363.	0.5	6
312	Methyl acrylatepolymerizations in the presence of a copper/N₃S₃macrobicyclic cage in DMSO at 25 Â°C. Polymer Chemistry, 2010, 1, 207-212.	1.9	6
313	Unraveling the Factors Behind the Efficiency of Hydrogen Evolution in Endohedrally Doped C₆₀ Structures via Ab Initio Calculations and Insights from Machine Learning Models. Advanced Theory and Simulations, 2019, 2, 1800202.	1.3	6
314	Huge Lithium Storage in 2D Bilayer Structures with Point Defects. Journal of Physical Chemistry C, 2021, 125, 23597-23603.	1.5	6
315	Recent developments in the quantum dynamical characterization of unimolecular resonances. Physical Chemistry Chemical Physics, 2004, 6, 884.	1.3	5
316	Molecular dynamic simulations of interactions between LDH and NO3â˜ intercalates in aqueous solution. Journal of Physics and Chemistry of Solids, 2008, 69, 1044-1047.	1.9	5
317	Tuning conductivity and magnetism in isopolar oxide superlattices via compressive and tensile strain: A case study of SrVO3/SrMnO3 and SrCrO3/SrMnO3 heterostructure. Journal of Applied Physics, 2016, 119, .	1.1	5
318	Electronic phase transitions under hydrostatic pressure in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaMnO</mml:mi><mml:mn>3</mml:mn></mml:msub></ bilayers sandwiched between<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaAlO</mml:mi><mml:mn>3</mml:mn></mml:msub></m Physical Review B, 2016, 93, .	1.1	5
319	New Insights on the Mechanism of Cyclization in Chromophore Maturation of Wild-Type Green Fluorescence Protein: A Computational Study. Journal of Physical Chemistry B, 2016, 120, 5386-5394.	1.2	5
320	Enhanced stability and stacking dependent magnetic/electronic properties of 2D monolayer FeTiO₃ on a Ti₂CO₂ substrate. Journal of Materials Chemistry C, 2019, 7, 15308-15314.	2.7	5
321	Analytical description of nanowires. I. Regular cross sections for zincblende and diamond structures. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 788-802.	0.5	5
322	Transition-state-theory calculations for reactions of O(3P) with halogenated olefins. Physical Chemistry Chemical Physics, 2004, 6, 5362.	1.3	4
323	Structural and electronic properties of diazonium functionalized (4, 4) single walled carbon nanotube: anab initiostudy. Molecular Simulation, 2006, 32, 1213-1217.	0.9	4
324	First-Principle Study of Atomic Hydrogen Interaction with a Fluorinated Corannulene Radical. Australian Journal of Chemistry, 2010, 63, 371.	0.5	4

#	Article	IF	Citations
325	Intrinsic ORR Activity Enhancement of Pt Atomic Sites by Engineering the d â€Band Center via Local Coordination Tuning. Angewandte Chemie, 2021, 133, 22082-22088.	1.6	4
326	INITIAL ROTATIONAL QUANTUM STATE EXCITATION AND ISOTOPIC EFFECTS FOR THE O(¹D)+HCl â† OH+Cl (OCl+H) REACTION. Journal of Theoretical and Computational Chemistry, 2009, 08, 1003-1024.	1.8	3
327	Half metallicity in a zigzag double-walled nanotube nanodot: An ab initio prediction. Chemical Physics Letters, 2009, 468, 257-259.	1.2	3
328	Dissociation dynamics ofHeRh2+in field-ion microscopy. Physical Review B, 2000, 61, 9419-9426.	1.1	2
329	The location of Ti atom in sodium alanate: an ab initio spin-polarised study. International Journal of Nanotechnology, 2007, 4, 564.	0.1	2
330	Quantum mechanical study of atomic hydrogen interaction with a fluorinated boron-substituted coronene radical. Journal of Physics Condensed Matter, 2009, 21, 144209.	0.7	2
331	Quantum Chemical Characterization of Low-Lying Excited States of an Aryl Peroxycarbonate: Mechanistic Implications for Photodissociation. Journal of Physical Chemistry A, 2010, 114, 4289-4295.	1.1	2
332	Nâ€Doped CsTaWO₆ as a New Photocatalyst for Hydrogen Production from Water Splitting Under Solar Irradiation. Advanced Functional Materials, 2011, 21, 125-125.	7.8	2
333	Fermi Level Determination for Charged Systems via Recursive Density of States Integration. Journal of Physical Chemistry Letters, 2018, 9, 4014-4019.	2.1	2
334	Cell Membrane Penetration without Pore Formation: Chameleonic Properties of Dendrimers in Response to Hydrophobic and Hydrophilic Environments. Advanced Theory and Simulations, 2020, 3, 1900152.	1.3	2
335	Activating Inert MXenes for Hydrogen Evolution Reaction via Anchored Metal Centers. Advanced Theory and Simulations, 2022, 5, .	1.3	2
336	Absorption and Photoluminescence of Silicon Nanocrystals Investigated by Excited State DFT: Role of Embedding Dielectric and Defects. Physica Status Solidi (B): Basic Research, 2022, 259, .	0.7	2
337	Circulants, symmetry and time-independent wavepacket scattering. Chemical Physics Letters, 1999, 312, 229-236.	1.2	1
338	Quantum dynamical characterization of unimolecular resonances. PhysChemComm, 2003, 6, 12-20.	0.8	1
339	A Lanczos-powered implementation of the Faber polynomial quantum time propagator for reaction probabilities. Chemical Physics Letters, 2004, 387, 277-282.	1.2	1
340	Molecular Modelling: All the Way from Atomistic Structure to Function in Complex Systems. Australian Journal of Chemistry, 2010, 63, 343.	0.5	1
341	CALCULATION OFHO₂DENSITY OF STATES ON THREE POTENTIAL ENERGY SURFACES. Journal of Theoretical and Computational Chemistry, 2010, 09, 653-665.	1.8	1
342	Electrocatalysts: In Operando Self-Healing of Perovskite Electrocatalysts: A Case Study of SrCoO3 for the Oxygen Evolution Reaction (Part. Part. Syst. Charact. 4/2017). Particle and Particle Systems Characterization, 2017, 34, .	1.2	1

#	Article	IF	Citations
343	Computational Materials Science: Discovering and Accelerating Future Technologies. Advanced Theory and Simulations, 2019, 2, 1900023.	1.3	1
344	Bridgeâ€•and Doubleâ€Bonded O and NH on Fully OHâ€•and NH 2 â€Terminated Silicon Nanocrystals: Ground and Excited State Properties. Physica Status Solidi (B): Basic Research, 2019, 256, 1800336.	0.7	1
345	Enhancing Cationic Drug Delivery with Polymeric Carriers: The Coulombâ€pH Switch Approach. Advanced Theory and Simulations, 2021, 4, 2000247.	1.3	1
346	On the Location of Boron in SiO 2 â€Embedded Si Nanocrystalsâ€”An Xâ€ray Absorption Spectroscopy and Density Functional Theory Study. Physica Status Solidi (B): Basic Research, 2021, 258, 2000623.	0.7	1
347	Application of inverse iteration to 2-dimensional master equations. , 1997, 18, 1004.		1
348	Unimolecular Reaction Dynamics: Theory and Experiments (Baer, Tomas; Hase, William L.). Journal of Chemical Education, 1998, 75, 1098.	1.1	0
349	Symmetry contaminations in reactive scattering through long-lived collision complexes. Chemical Physics, 2005, 308, 297-304.	0.9	0
350	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.	5.2	0
351	Bridgeâ€•and Doubleâ€Bonded O and NH on Fully OHâ€•and NH₂â€Terminated Silicon Nanocrystals: Ground and Excited State Properties (Phys. Status Solidi B 5/2019). Physica Status Solidi (B): Basic Research, 2019, 256, 1970023.	0.7	0
352	Design guidelines for transition metals as interstitial emitters in silicon nanocrystals to tune photoluminescence properties: zinc as biocompatible example. Nanoscale, 2020, 12, 19340-19349.	2.8	0
353	Hexagonal honeycomb silicon: Silicene. Series in Materials Science and Engineering, 2017, , 171-188.	0.1	0