Sean C Smith

List of Publications by Year in Descending Order

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	Regulating electron transfer over asymmetric low-spin Co(II) for highly selective electrocatalysis. *Chem Catalysis*, **2022**,		8
352	A single-Pt-atom-on-Ru-nanoparticle electrocatalyst for CO-resilient methanol oxidation. *Nature Catalysis*, **2022**, 5, 231-237	36.5	8
351	Modulating Pt-O-Pt atomic clusters with isolated cobalt atoms for enhanced hydrogen evolution catalysis.. *Nature Communications*, **2022**, 13, 2430	17.4	7
350	An Ultra-Long-Life Flexible Lithium-Sulfur Battery with Lithium Cloth Anode and Polysulfone-Functionalized Separator. *ACS Nano*, **2021**, 15, 1358-1369	16.7	19
349	Isolated copper-tin atomic interfaces tuning electrocatalytic CO conversion. *Nature Communications*, **2021**, 12, 1449	17.4	36
348	Template-Directed Rapid Synthesis of Pd-Based Ultrathin Porous Intermetallic Nanosheets for Efficient Oxygen Reduction. *Angewandte Chemie*, **2021**, 133, 11037-11044	3.6	4
347	Turning Low-Nanoscale Intrinsic Silicon Highly Electron-Conductive by SiO Coating. *ACS Applied Materials & Interfaces*, **2021**, 13, 20479-20488	9.5	1
346	Template-Directed Rapid Synthesis of Pd-Based Ultrathin Porous Intermetallic Nanosheets for Efficient Oxygen Reduction. *Angewandte Chemie - International Edition*, **2021**, 60, 10942-10949	16.4	35
345	On the Location of Boron in SiO2-Embedded Si NanocrystalsÂ An X-ray Absorption Spectroscopy and Density Functional Theory Study. *Physica Status Solidi (B): Basic Research*, **2021**, 258, 2000623	1.3	
344	Tailored Brownmillerite Oxide Catalyst with Multiple Electronic Functionalities Enables Ultrafast Water Oxidation. *Chemistry of Materials*, **2021**, 33, 5233-5241	9.6	19
343	Defect Engineering in Graphene-Confined Single-Atom Iron Catalysts for Room-Temperature Methane Conversion. *Journal of Physical Chemistry C*, **2021**, 125, 12628-12635	3.8	8
342	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	10	2
341	Enhancing Cationic Drug Delivery with Polymeric Carriers: The Coulomb-pH Switch Approach. *Advanced Theory and Simulations*, **2021**, 4, 2000247	3.5	1
340	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	13	2
339	Atomically Dispersed Indium Sites for Selective CO Electroreduction to Formic Acid. *ACS Nano*, **2021**, 15, 5671-5678	16.7	38
338	A molecular-level strategy to boost the mass transport of perovskite electrocatalyst for enhanced oxygen evolution. *Applied Physics Reviews*, **2021**, 8, 011407	17.3	12
337	Intrinsic ORR Activity Enhancement of Pt Atomic Sites by Engineering the d-Band Center via Local Coordination Tuning. *Angewandte Chemie*, **2021**, 133, 22082-22088	3.6	0

336	Controllable CO electrocatalytic reduction via ferroelectric switching on single atom anchored InSe monolayer. *Nature Communications*, **2021**, 12, 5128	17.4	30
335	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
334	Sulfur-Dopant-Promoted Electroreduction of CO over Coordinatively Unsaturated Ni-N Moieties. *Angewandte Chemie - International Edition*, **2021**, 60, 23342-23348	16.4	14
333	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
332	Phosphine vapor-assisted construction of heterostructured Ni2P/NiTe2 catalysts for efficient hydrogen evolution. *Energy and Environmental Science*, **2020**, 13, 1799-1807	35.4	56
331	Implanting Ni-O-VOx sites into Cu-doped Ni for low-overpotential alkaline hydrogen evolution. *Nature Communications*, **2020**, 11, 2720	17.4	65
330	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	
329	Non-equilibrium dynamics, materials and structures for hot carrier solar cells: a detailed review. *Semiconductor Science and Technology*, **2020**, 35, 073002	1.8	11
328	Boosting oxygen evolution reaction by activation of lattice-oxygen sites in layered Ruddlesden-Popper oxide. *EcoMat*, **2020**, 2, e12021	9.4	24
327	Vanadium Oxide Clusters Decorated Metallic Cobalt Catalyst for Active Alkaline Hydrogen Evolution. *Cell Reports Physical Science*, **2020**, 1, 100275	6.1	2
326	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
325	Stacking-Dependent Interlayer Magnetic Coupling in 2D CrI3/CrGeTe3 Nanostructures for Spintronics. *ACS Applied Nano Materials*, **2020**, 3, 1282-1288	5.6	27
324	Facile CO Oxidation on Oxygen-functionalized MXenes via the Mars-van Krevelen Mechanism. *ChemCatChem*, **2020**, 12, 1007-1012	5.2	2
323	Tungsten Oxide/Carbide Surface Heterojunction Catalyst with High Hydrogen Evolution Activity. *ACS Energy Letters*, **2020**, 5, 3560-3568	20.1	27
322	Efficient Water Splitting Actualized through an Electrochemistry-Induced Hetero-Structured Antiperovskite/(Oxy)Hydroxide Hybrid. *Small*, **2020**, 16, e2006800	11	13
321	Surface Reconstruction of Ultrathin Palladium Nanosheets during Electrocatalytic CO2 Reduction. *Angewandte Chemie*, **2020**, 132, 21677-21682	3.6	20
320	Surface Reconstruction of Ultrathin Palladium Nanosheets during Electrocatalytic CO Reduction. *Angewandte Chemie - International Edition*, **2020**, 59, 21493-21498	16.4	50
319	Confinement of Ionic Liquids at Single-Ni-Sites Boost Electroreduction of CO2 in Aqueous Electrolytes. *ACS Catalysis*, **2020**, 10, 13171-13178	13.1	27

318	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	
317	Direct insights into the role of epoxy groups on cobalt sites for acidic HO production. *Nature Communications*, **2020**, 11, 4181	17.4	73
316	Unusual synergistic effect in layered Ruddlesden-Popper oxide enables ultrafast hydrogen evolution. *Nature Communications*, **2019**, 10, 149	17.4	116
315	A Janus MoSSe monolayer: a superior and strain-sensitive gas sensing material. *Journal of Materials Chemistry A*, **2019**, 7, 1099-1106	13	106
314	Charge-controlled switchable H2 storage on conductive borophene nanosheet. *International Journal of Hydrogen Energy*, **2019**, 44, 20150-20157	6.7	17
313	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
312	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
311	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	
310	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
309	Unraveling Photocatalytic Mechanism and Selectivity in PET-RAFT Polymerization. *Advanced Theory and Simulations*, **2019**, 2, 1900038	3.5	21
308	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
307	Computational Materials Science: Discovering and Accelerating Future Technologies. *Advanced Theory and Simulations*, **2019**, 2, 1900023	3.5	0
306	Isolated Diatomic Ni-Fe Metal-Nitrogen Sites for Synergistic Electroreduction of CO. *Angewandte Chemie - International Edition*, **2019**, 58, 6972-6976	16.4	406
305	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	3.5	3
304	Versatile electrocatalytic processes realized by Ni, Co and Fe alloyed core coordinated carbon shells. *Journal of Materials Chemistry A*, **2019**, 7, 12154-12165	13	22
303	Isolated Diatomic Ni-Fe Metal□Nitrogen Sites for Synergistic Electroreduction of CO2. *Angewandte Chemie*, **2019**, 131, 7046-7050	3.6	42
302	Just add sugar for´carbohydrate induced self-assembly of curcumin. *Nature Communications*, **2019**, 10, 582	17.4	30
301	Bridge- and Double-Bonded O and NH on Fully OH- and NH2-Terminated Silicon Nanocrystals: Ground and Excited State Properties. *Physica Status Solidi (B): Basic Research*, **2019**, 256, 1800336	1.3	0

300	Super-Exchange Interaction Induced Overall Optimization in Ferromagnetic Perovskite Oxides Enables Ultrafast Water Oxidation. *Small*, **2019**, 15, e1903120	11	43
299	Cooperative defect-enriched SiO2 for oxygen activation and organic dehydrogenation. *Journal of Catalysis*, **2019**, 376, 168-179	7.3	10
298	Antipoisoning Nickel□arbon Electrocatalyst for Practical Electrochemical CO2 Reduction to CO. *ACS Applied Energy Materials*, **2019**, 2, 8002-8009	6.1	26
297	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	7.1	2
296	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	1.8	3
295	Light-Induced Synergistic Multidefect Sites on TiO2/SiO2 Composites for Catalytic Dehydrogenation. *ACS Catalysis*, **2019**, 9, 2674-2684	13.1	27
294	Electronic Structure Shift of Deeply Nanoscale Silicon by SiO2 versus Si3N4 Embedding as an Alternative to Impurity Doping. *Physical Review Applied*, **2019**, 12,	4.3	6
293	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	3.5	22
292	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
291	Oxygen Electrocatalysis at Mn-O -C Hybrid Heterojunction: An Electronic Synergy or Cooperative Catalysis?. *ACS Applied Materials & Interfaces*, **2019**, 11, 706-713	9.5	6
290	Synthesis, optical properties and theoretical modelling of discrete emitting states in doped silicon nanocrystals for bioimaging. *Nanoscale*, **2018**, 10, 15600-15607	7.7	10
289	SiO2 Modulation Doping for Si: Acceptor Candidates. *Physical Review Applied*, **2018**, 10,	4.3	6
288	Intrinsic ultrasmall nanoscale silicon turns n-/p-type with SiO/SiN-coating. *Beilstein Journal of Nanotechnology*, **2018**, 9, 2255-2264	3	11
287	Processable Surface Modification of Nickel-Heteroatom (N, S) Bridge Sites for Promoted Alkaline Hydrogen Evolution. *Angewandte Chemie*, **2018**, 131, 471	3.6	4
286	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
285	Extraordinary water adsorption characteristics of graphene oxide. *Chemical Science*, **2018**, 9, 5106-5111	9.4	72
284	Fermi Level Determination for Charged Systems via Recursive Density of States Integration. *Journal of Physical Chemistry Letters*, **2018**, 9, 4014-4019	6.4	1
283	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	19.4	13

282	On the mechanism of gas adsorption for pristine, defective and functionalized graphene. *Physical Chemistry Chemical Physics*, **2017**, 19, 6051-6056	3.6	51
281	Light, Catalyst, Activation: Boosting Catalytic Oxygen Activation Using a Light Pretreatment Approach. *ACS Catalysis*, **2017**, 7, 3644-3653	13.1	17
280	Modulation Doping of Silicon using Aluminium-induced Acceptor States in Silicon Dioxide. *Scientific Reports*, **2017**, 7, 46703	4.9	23
279	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,	3.1	1
278	The origin of low workfunctions in OH terminated MXenes. *Nanoscale*, **2017**, 9, 7016-7020	7.7	35
277	The mechanism of oxidation in chromophore maturation of wild-type green fluorescent protein: a theoretical study. *Physical Chemistry Chemical Physics*, **2017**, 19, 12942-12952	3.6	7
276	Understanding the Charge Transfer at the Interface of Electron Donors and Acceptors: TTF-TCNQ as an Example. *ACS Applied Materials & Interfaces*, **2017**, 9, 27266-27272	9.5	9
275	Borophene as a Promising Material for Charge-Modulated Switchable CO Capture. *ACS Applied Materials & Interfaces*, **2017**, 9, 19825-19830	9.5	62
274	The controlled disassembly of mesostructured perovskites as an avenue to fabricating high performance nanohybrid catalysts. *Nature Communications*, **2017**, 8, 15553	17.4	52
273	In Operando Self-Healing of Perovskite Electrocatalysts: A Case Study of SrCoO3 for the Oxygen Evolution Reaction. *Particle and Particle Systems Characterization*, **2017**, 34, 1600280	3.1	9
272	Computational design of two-dimensional nanomaterials for charge modulated CO2/H2 capture and/or storage. *Energy Storage Materials*, **2017**, 8, 169-183	19.4	21
271	Charge-modulated CO2 capture. *Current Opinion in Electrochemistry*, **2017**, 4, 118-123	7.2	6
270	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	6.9	13
269	Nitrogen Doped Carbon Nanosheets Coupled Nickel–Carbon Pyramid Arrays Toward Efficient Evolution of Hydrogen. *Advanced Sustainable Systems*, **2017**, 1, 1700032	5.9	9
268	Hexagonal honeycomb silicon: Silicene. *Series in Materials Science and Engineering*, **2017**, 171-188		
267	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
266	Formation and Migration of Oxygen Vacancies in SrCoO3 and Their Effect on Oxygen Evolution Reactions. *ACS Catalysis*, **2016**, 6, 5565-5570	13.1	66
265	Interfacing BiVO with Reduced Graphene Oxide for Enhanced Photoactivity: A Tale of Facet Dependence of Electron Shuttling. *Small*, **2016**, 12, 5295-5302	11	56

264	Electronic phase transitions under hydrostatic pressure in LaMnO3 (111) bilayers sandwiched between LaAlO3. *Physical Review B*, **2016**, 93,	3.3	5
263	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
262	High-mobility anisotropic transport in few-layer □B films. *Nanoscale*, **2016**, 8, 20111-20117	7.7	12
261	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, 5732-43	3.4	17
260	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, 5386-94	3.4	5
259	Charge-modulated permeability and selectivity in graphdiyne for hydrogen purification. *Molecular Simulation*, **2016**, 42, 573-579	2	18
258	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, 075301	2.5	3
257	Materials design for electrocatalytic carbon capture. *APL Materials*, **2016**, 4, 053202	5.7	18
256	Mobile Polaronic States in □MoO3: An ab Initio Investigation of the Role of Oxygen Vacancies and Alkali Ions. *ACS Applied Materials & Interfaces*, **2016**, 8, 10911-7	9.5	40
255	First-Principle Framework for Total Charging Energies in Electrocatalytic Materials and Charge-Responsive Molecular Binding at Gas-Surface Interfaces. *ACS Applied Materials & Interfaces*, **2016**, 8, 10897-903	9.5	16
254	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	2.3	21
253	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	
252	High activity and durability of novel perovskite electrocatalysts for water oxidation. *Materials Horizons*, **2015**, 2, 495-501	14.4	119
251	Phosphorene: Fabrication, Properties, and Applications. *Journal of Physical Chemistry Letters*, **2015**, 6, 2794-805	6.4	545
250	The mechanism of dehydration in chromophore maturation of wild-type green fluorescent protein: A theoretical study. *Chemical Physics Letters*, **2015**, 631-632, 42-46	2.5	8
249	Structural and Electronic Properties of Layered Arsenic and Antimony Arsenide. *Journal of Physical Chemistry C*, **2015**, 119, 6918-6922	3.8	184
248	H2 purification by functionalized graphdiyne □role of nitrogen doping. *Journal of Materials Chemistry A*, **2015**, 3, 6767-6771	13	56
247	Anisotropic Ripple Deformation in Phosphorene. *Journal of Physical Chemistry Letters*, **2015**, 6, 1509-13	6.4	88

246	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
245	Charge Modulation in Graphitic Carbon Nitride as a Switchable Approach to High-Capacity Hydrogen Storage. *ChemSusChem*, **2015**, 8, 3626-31	8.3	27
244	Encapsulated Silicene: A Robust Large-Gap Topological Insulator. *ACS Applied Materials & Interfaces*, **2015**, 7, 19226-33	9.5	28
243	Controlling molecular ordering in solution-state conjugated polymers. *Nanoscale*, **2015**, 7, 15134-41	7.7	11
242	Layered Graphene-Hexagonal BN Nanocomposites: Experimentally Feasible Approach to Charge-Induced Switchable CO2 Capture. *ChemSusChem*, **2015**, 8, 2987-93	8.3	37
241	Introduction to Computational Pharmaceutics **2015**, 1-5		3
240	Molecular Modeling of Layered Double Hydroxide Nanoparticles for Drug Delivery **2015**, 197-216		
239	Conductive Graphitic Carbon Nitride as an Ideal Material for Electrocatalytically Switchable CO2 Capture. *Scientific Reports*, **2015**, 5, 17636	4.9	48
238	Orbital engineering of two-dimensional materials with hydrogenation: A realization of giant gap and strongly correlated topological insulators. *Physical Review B*, **2015**, 92,	3.3	14
237	Quantum spin Hall effect and topological phase transition in two-dimensional square transition-metal dichalcogenides. *Physical Review B*, **2015**, 92,	3.3	106
236	Peculiarity of Two Thermodynamically-Stable Morphologies and Their Impact on the Efficiency of Small Molecule Bulk Heterojunction Solar Cells. *Scientific Reports*, **2015**, 5, 13407	4.9	15
235	Tetragonal bismuth bilayer: a stable and robust quantum spin hall insulator. *2D Materials*, **2015**, 2, 045010	5.9	29
234	The isotopic effects of deuteration on optoelectronic properties of conducting polymers. *Nature Communications*, **2014**, 5, 3180	17.4	82
233	Theoretical Predictions of Freestanding Honeycomb Sheets of Cadmium Chalcogenides. *Journal of Physical Chemistry C*, **2014**, 118, 16236-16245	3.8	33
232	Growth and Electrochemical Characterization of Carbon Nanospike Thin Film Electrodes. *Journal of the Electrochemical Society*, **2014**, 161, H558-H563	3.9	22
231	Exceptional Optoelectronic Properties of Hydrogenated Bilayer Silicene. *Physical Review X*, **2014**, 4,	9.1	26
230	Electrocatalytically switchable CO2 capture: first principle computational exploration of carbon nanotubes with pyridinic nitrogen. *ChemSusChem*, **2014**, 7, 435-41	8.3	55
229	Weak competing interactions control assembly of strongly bonded TCNQ ionic acceptor molecules on silver surfaces. *Physical Review B*, **2014**, 90,	3.3	10

228	Modelling carbon membranes for gas and isotope separation. *Physical Chemistry Chemical Physics*, **2013**, 15, 4832-43	3.6	84
227	Porous Graphene and Nanomeshes **2013**, 129-151		1
226	High-performance polymer photovoltaics based on rationally designed fullerene acceptors. *Solar Energy Materials and Solar Cells*, **2013**, 118, 171-178	6.4	23
225	Structures, Energetics, and Electronic Properties of Layered Materials and Nanotubes of Cadmium Chalcogenides. *Journal of Physical Chemistry C*, **2013**, 117, 25817-25825	3.8	19
224	Charge-dependent dynamics of a polyelectrolyte dendrimer and its correlation with invasive water. *Journal of the American Chemical Society*, **2013**, 135, 5111-7	16.4	10
223	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
222	Colloidal Semiconductor Nanowires **2013**, 65-104		
221	Density functional theory study on adsorption of Pt nanoparticle on graphene. *International Journal of Hydrogen Energy*, **2013**, 38, 6283-6287	6.7	16
220	Chemically modified ribbon edge stimulated H2 dissociation: a first-principles computational study. *Physical Chemistry Chemical Physics*, **2013**, 15, 8054-7	3.6	22
219	Charge carrier exchange at chemically modified graphene edges: a density functional theory study. *Journal of Materials Chemistry*, **2012**, 22, 8321		21
218	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, 1426-36	3.4	18
217	Structured water in polyelectrolyte dendrimers: understanding small angle neutron scattering results through atomistic simulation. *Journal of Chemical Physics*, **2012**, 136, 144901	3.9	18
216	Methane activation on Fe4 cluster: A density functional theory study. *Chemical Physics Letters*, **2012** , 550, 41-46	2.5	17
215	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	3.8	29
214	Strong Interaction between Gold and Anatase TiO2(001) Predicted by First Principle Studies. *Journal of Physical Chemistry C*, **2012**, 116, 3524-3531	3.8	48
213	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	2	7
212	Molecular dynamics and neutron scattering study of the dependence of polyelectrolyte dendrimer conformation on counterion behavior. *Journal of Chemical Physics*, **2012**, 137, 064902	3.9	7
211	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

210	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
209	How to achieve maximum charge carrier loading on heteroatom-substituted graphene nanoribbon edges: density functional theory study. *Journal of Materials Chemistry*, **2012**, 22, 13751		21
208	First-principles prediction of metal-free magnetism and intrinsic half-metallicity in graphitic carbon nitride. *Physical Review Letters*, **2012**, 108, 197207	7.4	234
207	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
206	Isomerization mechanism of the HcRed fluorescent protein chromophore. *Physical Chemistry Chemical Physics*, **2012**, 14, 11413-24	3.6	20
205	Theoretical study of two states reactivity of methane activation on iron atom and iron dimer. *Fuel*, **2012**, 96, 291-297	7.1	22
204	Hydrotalcite Intercalated siRNA: Computational Characterization of the Interlayer Environment. *Pharmaceutics*, **2012**, 4, 296-313	6.4	6
203	Graphdiyne: a versatile nanomaterial for electronics and hydrogen purification. *Chemical Communications*, **2011**, 47, 11843-5	5.8	289
202	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
201	Cobalt-doped cadmium selenide colloidal nanowires. *Chemical Communications*, **2011**, 47, 11894-6	5.8	15
200	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
199	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	3.8	6
198	Lattice distortion oriented angular self-assembly of monolayer titania sheets. *Journal of the American Chemical Society*, **2011**, 133, 695-7	16.4	43
197	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
196	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
195	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
194	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
193	Photocatalytic Hydrogen Production from Water Using N-Doped Ba5Ta4O15 under Solar Irradiation. *Journal of Physical Chemistry C*, **2011**, 115, 15674-15678	3.8	77

192	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
191	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
190	N-Doped CsTaWO6 as a New Photocatalyst for Hydrogen Production from Water Splitting Under Solar Irradiation. *Advanced Functional Materials*, **2011**, 21, 125-125	15.6	2
189	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, 13645-55	3.6	25
188	Energy dependent dynamics of the O(1D) + HCl reaction: a quantum, quasiclassical and statistical study. *Physical Chemistry Chemical Physics*, **2011**, 13, 8502-14	3.6	12
187	Nitrogen doping in ion-exchangeable layered tantalate towards visible-light induced water oxidation. *Chemical Communications*, **2011**, 47, 6293-5	5.8	57
186	Kinetic modelling of molecular hydrogen transport in microporous carbon materials. *Physical Chemistry Chemical Physics*, **2011**, 13, 7834-44	3.6	27
185	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
184	Bandgap narrowing of titanium oxide nanosheets: homogeneous doping of molecular iodine for improved photoreactivity. *Journal of Materials Chemistry*, **2011**, 21, 14672		27
183	Multiple hydrogen-bonded complexes based on 2-ureido-4[1H]-pyrimidinone: a theoretical study. *Journal of Physical Chemistry B*, **2011**, 115, 11053-62	3.4	22
182	Interaction of Water with the Fluorine-Covered Anatase TiO2 (001) Surface. *Journal of Physical Chemistry C*, **2011**, 115, 17092-17096	3.8	20
181	Hydrogen Incorporation and Storage in Well-Defined Nanocrystals of Anatase Titanium Dioxide. *Journal of Physical Chemistry C*, **2011**, 115, 25590-25594	3.8	92
180	Molecular modeling of hydrotalcite structure intercalated with transition metal oxide anions: CrO4(2-) and VO4(3-). *Journal of Physical Chemistry A*, **2011**, 115, 13673-83	2.8	10
179	Improved visible light absorption of HTaWO6 induced by nitrogen doping: An experimental and theoretical study. *Chemical Physics Letters*, **2011**, 501, 427-430	2.5	8
178	Quantum calculations for the S(1D)+H2reaction employing the ground adiabatic electronic state. *Physica Scripta*, **2011**, 84, 028102	2.6	13
177	CALCULATION OF HO2 DENSITY OF STATES ON THREE POTENTIAL ENERGY SURFACES. *Journal of Theoretical and Computational Chemistry*, **2010**, 09, 653-665	1.8	1
176	First-Principle Study of Atomic Hydrogen Interaction with a Fluorinated Corannulene Radical. *Australian Journal of Chemistry*, **2010**, 63, 371	1.2	4
175	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

174	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
173	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
172	QM/MM studies of structural and energetic properties of the far-red fluorescent protein HcRed. *Physical Chemistry Chemical Physics*, **2010**, 12, 2450-8	3.6	28
171	The mechanism of cyclization in chromophore maturation of green fluorescent protein: a theoretical study. *Journal of Physical Chemistry B*, **2010**, 114, 9698-705	3.4	14
170	Oxygen vacancy induced structural variations of exfoliated monolayer MnO2 sheets. *Physical Review B*, **2010**, 81,	3.3	23
169	Quantum chemical characterization of low-lying excited states of an aryl peroxycarbonate: mechanistic implications for photodissociation. *Journal of Physical Chemistry A*, **2010**, 114, 4289-95	2.8	2
168	Methyl acrylate polymerizations in the presence of a copper/N3S3 macrobicyclic cage in DMSO at 25 °C. *Polymer Chemistry*, **2010**, 1, 207-212	4.9	5
167	Nanosized anatase TiO2 single crystals for enhanced photocatalytic activity. *Chemical Communications*, **2010**, 46, 755-7	5.8	375
166	Computer Modeling Study for Intercalation of Drug Heparin into Layered Double Hydroxide. *Journal of Physical Chemistry C*, **2010**, 114, 12618-12629	3.8	15
165	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
164	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
163	Unique electronic structure induced high photoreactivity of sulfur-doped graphitic C3N4. *Journal of the American Chemical Society*, **2010**, 132, 11642-8	16.4	1597
162	A density functional theory study of CO2 and N2 adsorption on aluminium nitride single walled nanotubes. *Journal of Materials Chemistry*, **2010**, 20, 10426		54
161	Exact and truncated Coriolis coupling calculations for the S(1D)+HD reaction employing the ground adiabatic electronic state. *Physical Chemistry Chemical Physics*, **2010**, 12, 12711-8	3.6	27
160	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
159	Structural and Relaxation Effects in Proton Wire Energetics: Model Studies of the Green Fluorescent Protein Photocycle. *Australian Journal of Chemistry*, **2010**, 63, 363	1.2	6
158	Molecular Modelling: All the Way from Atomistic Structure to Function in Complex Systems. *Australian Journal of Chemistry*, **2010**, 63, 343	1.2	1
157	Titania-water interactions: a review of theoretical studies. *Journal of Materials Chemistry*, **2010**, 20, 10319		228

156	Synthesis and Characterization of Colloidal Core–Shell Semiconductor Nanowires. *European Journal of Inorganic Chemistry*, **2010**, 2010, 4325-4331	2.3	34
155	Theoretical Studies of Green and Red Fluorescent Proteins **2010**, 815-837		1
154	Diluted magnetic semiconductor nanowires prepared by the solution-liquid-solid method. *Angewandte Chemie - International Edition*, **2010**, 49, 2777-81	16.4	44
153	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
152	Formation energies of low-indexed surfaces of tin dioxide terminated by nonmetals. *Solid State Communications*, **2010**, 150, 957-960	1.6	6
151	INITIAL ROTATIONAL QUANTUM STATE EXCITATION AND ISOTOPIC EFFECTS FOR THE O(1D)+HCl -> OH+Cl (OCl+H) REACTION. *Journal of Theoretical and Computational Chemistry*, **2009**, 08, 1003-1024	1.8	3
150	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, 4388-91	1.3	8
149	Quantum mechanical study of atomic hydrogen interaction with a fluorinated boron-substituted coronene radical. *Journal of Physics Condensed Matter*, **2009**, 21, 144209	1.8	1
148	Lithium-Catalyzed Dehydrogenation of Ammonia Borane within Mesoporous Carbon Framework for Chemical Hydrogen Storage. *Advanced Functional Materials*, **2009**, 19, 265-271	15.6	148
147	Numerical solution methods for large, difficult kinetic master equations. *Theoretical Chemistry Accounts*, **2009**, 124, 303-317	1.9	13
146	Half metallicity in a zigzag double-walled nanotube nanodot: An ab initio prediction. *Chemical Physics Letters*, **2009**, 468, 257-259	2.5	3
145	First principle studies of zigzag AlN nanoribbon. *Chemical Physics Letters*, **2009**, 469, 183-185	2.5	83
144	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
143	Intercalation of Sulfonate into Layered Double Hydroxide: Comparison of Simulation with Experiment. *Journal of Physical Chemistry C*, **2009**, 113, 559-566	3.8	38
142	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
141	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
140	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
139	The effect of Fe doping on adsorption of CO2/N2 within carbon nanotubes: a density functional theory study with dispersion corrections. *Nanotechnology*, **2009**, 20, 375701	3.4	19

138	Efficient Promotion of Anatase TiO2 Photocatalysis via Bifunctional Surface-Terminating TiOBN Structures. *Journal of Physical Chemistry C*, **2009**, 113, 12317-12324	3.8	109
137	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
136	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
135	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
134	Flexibility of Short-Strand RNA in Aqueous Solution as Revealed by Molecular Dynamics Simulation: Are A-RNA and A□-RNA Distinct Conformational Structures?. *Australian Journal of Chemistry*, **2009**, 62, 1054	1.2	7
133	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	6
132	Reducible disulfide-based non-viral gene delivery systems. *Mini-Reviews in Medicinal Chemistry*, **2009**, 9, 1242-50	3.2	11
131	Anatase TiO2 single crystals with a large percentage of reactive facets. *Nature*, **2008**, 453, 638-41	50.4	3391
130	Effect of dimerization on vibrational spectra of eumelanin precursors. *Photochemistry and Photobiology*, **2008**, 84, 613-9	3.6	12
129	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	3.9	31
128	Computational study of methyl derivatives of ammonia borane for hydrogen storage. *Physical Chemistry Chemical Physics*, **2008**, 10, 6104-6	3.6	12
127	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, 7947-60	2.8	14
126	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
125	Quantum calculation of ro-vibrational states: methodology and DOCl application results. *Journal of Physical Chemistry A*, **2008**, 112, 4141-7	2.8	5
124	Quantum dynamical study of the O(1D)+HCl reaction employing three electronic state potential energy surfaces. *Journal of Chemical Physics*, **2008**, 128, 014308	3.9	21
123	The role of V2O5 on the dehydrogenation and hydrogenation in magnesium hydride: An ab initio study. *Applied Physics Letters*, **2008**, 92, 163106	3.4	21
122	Half metallicty in finite-length zigzag single walled carbon nanotube: A first-principle prediction. *Applied Physics Letters*, **2008**, 93, 073101	3.4	31
121	Molecular dynamic simulations of interactions between LDH and NO3□intercalates in aqueous solution. *Journal of Physics and Chemistry of Solids*, **2008**, 69, 1044-1047	3.9	4

120	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
119	Role of Lithium Vacancies in Accelerating the Dehydrogenation Kinetics on a LiBH4(010) Surface: An Ab Initio Study. *Journal of Physical Chemistry C*, **2007**, 111, 12124-12128	3.8	10
118	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, 452-8	3.6	23
117	First-Principle Studies of the Formation and Diffusion of Hydrogen Vacancies in Magnesium Hydride. *Journal of Physical Chemistry C*, **2007**, 111, 8360-8365	3.8	56
116	OH-initiated oxidation of toluene. 2. Master equation simulation of toluene oxide isomerization. *Journal of Physical Chemistry A*, **2007**, 111, 3691-6	2.8	13
115	Metallic and carbon nanotube-catalyzed coupling of hydrogenation in magnesium. *Journal of the American Chemical Society*, **2007**, 129, 15650-4	16.4	114
114	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
113	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
112	Formation of single-walled carbon nanotube via the interaction of graphene nanoribbons: ab initio density functional calculations. *Nano Letters*, **2007**, 7, 3349-54	11.5	22
111	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
110	Addition of diazomethane to armchair single-walled carbon nanotubes and their reaction sequences: A computational study. *Chemical Physics Letters*, **2007**, 436, 218-223	2.5	17
109	First-principle studies of electronic structure and C-doping effect in boron nitride nanoribbon. *Chemical Physics Letters*, **2007**, 447, 181-186	2.5	158
108	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	2.5	29
107	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
106	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
105	The location of Ti atom in sodium alanate: an ab initio spin-polarised study. *International Journal of Nanotechnology*, **2007**, 4, 564	1.5	2
104	State-to-state reaction probabilities for the H+O2(v,j)-->O+OH(v',j') reaction on three potential energy surfaces. *Journal of Chemical Physics*, **2007**, 127, 064316	3.9	28
103	A structural basis for the pH-dependent increase in fluorescence efficiency of chromoproteins. *Journal of Molecular Biology*, **2007**, 368, 998-1010	6.5	23

102	Vacancy mediated desorption of hydrogen from a sodium alanate surface: An ab initio spin-polarized study. *Applied Physics Letters*, **2007**, 90, 143119	3.4	12
101	Structural and electronic properties of diazonium functionalized (4, 4) single walled carbon nanotube: an ab initio study. *Molecular Simulation*, **2006**, 32, 1213-1217	2	4
100	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
99	Molecular orbital calculations of two-electron states for P-donor solid-state spin qubits. *Physical Review B*, **2006**, 73,	3.3	14
98	Mg-based nanocomposites with high capacity and fast kinetics for hydrogen storage. *Journal of Physical Chemistry B*, **2006**, 110, 11697-703	3.4	80
97	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
96	Catalytic effects of subsurface carbon in the chemisorption of hydrogen on a Mg(0001) surface: an ab-initio study. *Journal of Physical Chemistry B*, **2006**, 110, 1814-9	3.4	48
95	Mechanistic aspects of proton chain transfer: a computational study for the green fluorescent protein chromophore. *Journal of Physical Chemistry B*, **2006**, 110, 5084-93	3.4	23
94	HOCl Ro-vibrational bound-state calculations for nonzero total angular momentum. *Journal of Physical Chemistry A*, **2006**, 110, 5468-74	2.8	5
93	HO2 ro-vibrational bound-state calculations for large angular momentum: J = 30, 40, and 50. *Journal of Physical Chemistry A*, **2006**, 110, 3246-53	2.8	16
92	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	2.3	9
91	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	2.5	16
90	trans□is Isomerism and acylimine formation in DsRed chromophore models: Intrinsic rotation barriers. *Chemical Physics Letters*, **2006**, 426, 159-162	2.5	11
89	Ab initio studies of hydrogen desorption from low index magnesium hydride surface. *Surface Science*, **2006**, 600, 1854-1859	1.8	56
88	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
87	The 2.0 angstroms 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, 359-66	3.6	8
86	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
85	Van der Waals-corrected density functional theory: benchmarking for hydrogen-nanotube and nanotube-nanotube interactions. *Nanotechnology*, **2005**, 16, 2118-23	3.4	51

84	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
83	Symmetry contaminations in reactive scattering through long-lived collision complexes. *Chemical Physics*, **2005**, 308, 297-304	2.3	
82	Unimolecular rovibrational bound and resonance states for large angular momentum: J=20 calculations for HO2. *Journal of Chemical Physics*, **2005**, 123, 014308	3.9	13
81	Full S matrix calculation via a single real-symmetric Lanczos recursion: the Lanczos artificial boundary inhomogeneity method. *Journal of Chemical Physics*, **2004**, 120, 1161-3	3.9	8
80	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	1.8	8
79	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
78	Comparative study of hydrogen storage in Li- and K-doped carbon materials theoretically revisited. *Carbon*, **2004**, 42, 2509-2514	10.4	47
77	A Lanczos-powered implementation of the Faber polynomial quantum time propagator for reaction probabilities. *Chemical Physics Letters*, **2004**, 387, 277-282	2.5	1
76	On the microscopic mechanism of carbon gasification: A theoretical study. *Carbon*, **2004**, 42, 2921-2928	10.4	55
75	Recent developments in the quantum dynamical characterization of unimolecular resonances. *Physical Chemistry Chemical Physics*, **2004**, 6, 884	3.6	5
74	Iterative quantum computations of HO2 bound states and resonances for J = 4 and 5. *Physical Chemistry Chemical Physics*, **2004**, 6, 4240	3.6	10
73	Transition-state-theory calculations for reactions of O(3P) with halogenated olefins. *Physical Chemistry Chemical Physics*, **2004**, 6, 5362	3.6	4
72	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
71	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
70	Selecting Methods to Solve Multi-Well Master Equations. *Journal of Theoretical and Computational Chemistry*, **2003**, 02, 179-191	1.8	11
69	Quantum dynamical characterization of unimolecular resonances. *PhysChemComm*, **2003**, 6, 12-20		
68	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,	3.3	43
67	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	3.9	7

66	Fast, scalable master equation solution algorithms. IV. Lanczos iteration with diffusion approximation preconditioned iterative inversion. *Journal of Chemical Physics*, **2003**, 119, 12741-12748	3.9	8
65	Calculation of bound and resonance states of HO2 for nonzero total angular momentum. *Journal of Chemical Physics*, **2003**, 118, 10042-10050	3.9	21
64	Ab initio modelling of basal plane oxidation of graphenes and implications for modelling char combustion. *Carbon*, **2002**, 40, 2341-2349	10.4	41
63	A real symmetric Lanczos subspace implementation of quantum scattering using boundary inhomogeneities. *Chemical Physics Letters*, **2002**, 366, 390-397	2.5	10
62	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
61	Chebyshev real wave packet propagation: H+O2 (J=0) state-to-state reactive scattering calculations. *Journal of Chemical Physics*, **2002**, 117, 5174-5182	3.9	21
60	Prediction of absolute rate coefficients and product branching ratios for the C(3P)+allene reaction system. *Journal of Chemical Physics*, **2002**, 117, 7055-7067	3.9	7
59	Lanczos Subspace Time-Independent Wave Packet Calculations of S (1D) + H2Reactive Scattering. *Journal of Physical Chemistry A*, **2002**, 106, 6137-6142	2.8	13
58	Calculation of Resonances and Product State Distributions for the Unimolecular Dissociation of H2S. *Journal of Physical Chemistry A*, **2002**, 106, 6129-6136	2.8	5
57	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	4.2	13
56	Subspace wavepacket evolution with Newton polynomials. *Chemical Physics Letters*, **2001**, 336, 149-155	2.5	14
55	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	2.5	12
54	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	3.6	37
53	Calculation of product state distributions from resonance decay via Lanczos subspace filter diagonalization: Application to HO2. *Journal of Chemical Physics*, **2001**, 115, 5751-5758	3.9	30
52	Time-dependent master equation simulation of complex elementary reactions in combustion: application to the reaction of 1CH2 with C2H2 from 300-2000 K. *Faraday Discussions*, **2001**, 159-71; discussion 255-74	3.6	21
51	Solving the unimolecular master equation with a weighted subspace projection method. *Journal of Computational Chemistry*, **2000**, 21, 592-606	3.5	11
50	Dissociation dynamics of HeRh2+ in field-ion microscopy. *Physical Review B*, **2000**, 61, 9419-9426	3.3	2
49	A master equation model for bimolecular reaction via multi-well isomerizing intermediates. *Physical Chemistry Chemical Physics*, **2000**, 2, 793-803	3.6	32

48	Kinematic Factors in Transition State Theory with a Generalized Reaction Coordinate *Journal of Physical Chemistry A*, **2000**, 104, 10489-10499	2.8	10
47	Classical flux integrals in transition state theory: Generalized reaction coordinates. *Journal of Chemical Physics*, **1999**, 111, 1830-1842	3.9	22
46	Application of contracted distributed approximating functions to solving vibrational eigenvalue problems. *Journal of Chemical Physics*, **1999**, 110, 72-79	3.9	7
45	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	3.9	11
44	Circulants, symmetry and time-independent wavepacket scattering. *Chemical Physics Letters*, **1999**, 312, 229-236	2.5	1
43	Optimal spectral filtering in a finite subspace: a Lanczos-based implementation. *Physical Chemistry Chemical Physics*, **1999**, 1, 1311-1316	3.6	12
42	Removal of orthodontic bonding resin residues by CO2 laser radiation: surface effects. *Photomedicine and Laser Surgery*, **1999**, 17, 13-8		14
41	Calculation of quantum resonance energies and lifetimes via quasi-minimum residual filter diagonalization. *Chemical Physics Letters*, **1998**, 283, 69-76	2.5	36
40	The Elimination of Lanczos Ghosting Effects by MINRES Filter Diagonalization. *Journal of Computational Physics*, **1998**, 143, 484-494	4.1	22
39	Theoretical Study of the Reaction CH(2) + NO(2). 3. Determination of the Branching Ratios. *Journal of Physical Chemistry A*, **1998**, 102, 3358-3367	2.8	15
38	Unimolecular Reaction Dynamics: Theory and Experiments (Baer, Tomas; Hase, William L.). *Journal of Chemical Education*, **1998**, 75, 1098	2.4	
37	The simulation of outgoing-wave boundary conditions via a symmetrically damped, Hermitian Hamiltonian operator. *Journal of Chemical Physics*, **1997**, 107, 9985-9993	3.9	20
36	Restarted Krylov-space spectral filtering. *Journal of the Chemical Society, Faraday Transactions*, **1997**, 93, 861-869		15
35	Reversibility Relationship in Collision-Complex-Forming Bimolecular Reactions. *Journal of Physical Chemistry A*, **1997**, 101, 7311-7314	2.8	8
34	Multiple-Well Isomerization Diffusion Equation Solutions with a Shift and Invert Lanczos Algorithm. *Journal of Physical Chemistry A*, **1997**, 101, 5765-5769	2.8	20
33	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	3.9	27
32	The calculation of vibrational eigenstates by MINRES filter diagonalization. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1997**, 101, 400-406		92
31	Application of inverse iteration to 2-dimensional master equations. *Journal of Computational Chemistry*, **1997**, 18, 1004-1010	3.5	25

30	Calculation of the vibrational spectral density of NO2 via density correlation functions. *Chemical Physics Letters*, **1997**, 273, 55-61	2.5	12
29	Calculation of absolute spectral densities via stochastic estimators of tr{□(E - □)}. *Chemical Physics Letters*, **1997**, 278, 345-351	2.5	11
28	Application of inverse iteration to 2-dimensional master equations **1997**, 18, 1004		1
27	Full Iterative Solution of the Two-Dimensional Master Equation for Thermal Unimolecular Reactions. *The Journal of Physical Chemistry*, **1996**, 100, 7090-7096		42
26	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
25	On the calculation of absolute spectral densities. *Journal of Chemical Physics*, **1996**, 105, 4055-4064	3.9	13
24	Kinetics and Product Branching Ratios for the Reaction HCO + NO2. *The Journal of Physical Chemistry*, **1995**, 99, 7473-7481		23
23	Towards quantum mechanical characterization of the dissociation dynamics of ketene. *Faraday Discussions*, **1995**, 102, 17	3.6	12
22	A pseudo-spectral algorithm for the computation of transitional-mode eigenfunctions in loose transition states. *Chemical Physics Letters*, **1995**, 243, 359-366	2.5	10
21	Flux Factors in Variational Transition-State Theory. *The Journal of Physical Chemistry*, **1994**, 98, 6496-6504		13
20	A comparison of an experimental unimolecular lifetime distribution with Rice–Ramsperger–Kassel–Marcus theory. *Journal of Chemical Physics*, **1994**, 100, 5696-5705	3.9	10
19	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
18	Rapid algorithms for microcanonical variational Rice-Ramsperger-Kassel-Marcus theory. *The Journal of Physical Chemistry*, **1993**, 97, 7034-7039		28
17	Statistical modeling of capture, association, and exit-channel dynamics in the CH3+/CH3CN system. *Journal of Chemical Physics*, **1993**, 98, 1944-1956	3.9	20
16	Angular-momentum resolution in transitional-mode state counting for loose transition states. *Journal of Chemical Physics*, **1992**, 97, 2406-2416	3.9	44
15	Statistical modeling of ion–molecule electrostatic capture. *Journal of Chemical Physics*, **1992**, 97, 5451-5464	3.9	57
14	A convenient procedure for the synthesis of bis-steroidal pyrazines: models for the cephalostatins. *Journal of Organic Chemistry*, **1992**, 57, 6379-6380	4.2	46
13	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

12	Entropy barriers to proton transfer. *Journal of the American Chemical Society*, **1991**, 113, 862-869	16.4	39
11	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
10	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
9	The relationship between recombination, chemical activation and unimolecular dissociation rate coefficients. *Journal of Chemical Physics*, **1989**, 90, 4265-4273	3.9	55
8	The pressure dependence of ion–molecule association rate coefficients. *Journal of Chemical Physics* , **1989**, 90, 1630-1640	3.9	29
7	Microscopic reaction rates in ion/molecule reactions: effects of uncoupled modes. *The Journal of Physical Chemistry*, **1989**, 93, 8142-8148		21
6	Angular momentum conservation in unimolecular and recombination reactions. *International Journal of Chemical Kinetics*, **1988**, 20, 307-329	1.4	74
5	Angular momentum conservation in multichannel unimolecular reactions. *International Journal of Chemical Kinetics*, **1988**, 20, 979-990	1.4	34
4	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
3	Facet-dependent carrier dynamics of cuprous oxide regulating the photocatalytic hydrogen generation. *Materials Advances*,	3.3	3
2	Autocatalytic Surface Reduction-Assisted Synthesis of PtW Ultrathin Alloy Nanowires for Highly Efficient Hydrogen Evolution Reaction. *Advanced Energy Materials*,2103943	21.8	6
1	Activating Inert MXenes for Hydrogen Evolution Reaction via Anchored Metal Centers. *Advanced Theory and Simulations*,2100383	3.5	