William A Goddard

List of Publications by Year in Descending Order

645 papers	76,103 citations	130 h-index	258 g-index
653 ext. papers	83,955 ext. citations	8.3 avg, IF	8.16 L-index

#	Paper	IF	Citations
645	Complete inhibition of a polyol nucleation by a micromolar biopolymer additive.. *Cell Reports Physical Science*, **2022**, 3, 100723-100723	6.1	0
644	Au-activated N motifs in non-coherent cupric porphyrin metal organic frameworks for promoting and stabilizing ethylene production.. *Nature Communications*, **2022**, 13, 63	17.4	11
643	Biased Agonists Favoring Gs over Arrestin for Individualized Treatment of Obstructive Lung Disease.. *Journal of Personalized Medicine*, **2022**, 12,	3.6	1
642	Reactive scattering of water group ions on ice surfaces with relevance to Saturn's icy moons. *Icarus*, **2022**, 379, 114967	3.8	
641	First-Principles Molecular Dynamics in Metal-Halide Perovskites: Contrasting Generalized Gradient Approximation and Hybrid Functionals. *Journal of Physical Chemistry Letters*, **2021**, 11886-11893	6.4	4
640	Order-Tuned Deformability of Bismuth Telluride Semiconductors: An Energy-Dissipation Strategy for Large Fracture Strain. *ACS Applied Materials & Interfaces*, **2021**, 13, 57629-57637	9.5	
639	Structure, Energetics, and Spectra for the Oxygen Vacancy in Rutile: Prominence of the Ti-H-Ti Bond. *Journal of Physical Chemistry Letters*, **2021**, 12, 10175-10181	6.4	1
638	Reaction Mechanism and Energetics of Decomposition of Tetrakis(1,3-dimethyltetrazol-5-imidoperchloratomanganese(II)) from Quantum-Mechanics-based Reactive Dynamics. *Journal of the American Chemical Society*, **2021**, 143, 16960-16975	16.4	1
637	Synergic Effects in the Activation of the Sweet Receptor GPCR Heterodimer for Various Sweeteners Predicted Using Molecular Metadynamics Simulations. *Journal of Agricultural and Food Chemistry*, **2021**, 69, 12250-12261	5.7	1
636	Electrochemical Performance and Structures of Chromium and Molybdenum-Doped LixVOPO4 Predicted as Promising Cathodes for Next Generation Lithium-Ion Batteries. *Journal of Physical Chemistry C*, **2021**, 125, 275-282	3.8	1
635	Autobifunctional Mechanism of Jagged Pt Nanowires for Hydrogen Evolution Kinetics via End-to-End Simulation. *Journal of the American Chemical Society*, **2021**, 143, 5355-5363	16.4	7
634	Effects of High and Low Salt Concentrations in Electrolytes at Lithium-Metal Anode Surfaces Using DFT-ReaxFF Hybrid Molecular Dynamics Method. *Journal of Physical Chemistry Letters*, **2021**, 12, 2922-2929	6.4	12
633	Stabilizing Highly Active Ru Sites by Suppressing Lattice Oxygen Participation in Acidic Water Oxidation. *Journal of the American Chemical Society*, **2021**, 143, 6482-6490	16.4	38
632	Mechanistic Studies of Styrene Production from Benzene and Ethylene Using [(-C2H4)2Rh(OAc)]2 as Catalyst Precursor: Identification of a Bis-RhI Mono-CuII Complex As the Catalyst. *ACS Catalysis*, **2021**, 11, 5688-5702	13.1	3
631	Predicted Operando Polymerization at Lithium Anode via Boron Insertion. *ACS Energy Letters*, **2021**, 6, 2320-2327	20.1	7
630	CO reduction on pure Cu produces only H after subsurface O is depleted: Theory and experiment. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	11
629	Predictions of Chemical Shifts for Reactive Intermediates in CO Reduction under Conditions. *ACS Applied Materials & Interfaces*, **2021**, 13, 31554-31560	9.5	3

628	Artificial Intelligence and QM/MM with a Polarizable Reactive Force Field for Next-Generation Electrocatalysts. *Matter*, **2021**, 4, 195-216	12.7	16
627	London Dispersion Corrections to Density Functional Theory for Transition Metals Based on Fitting to Experimental Temperature-Programmed Desorption of Benzene Monolayers. *Journal of Physical Chemistry Letters*, **2021**, 12, 73-79	6.4	
626	Oxygen evolution reaction over catalytic single-site Co in a well-defined brookite TiO2 nanorod surface. *Nature Catalysis*, **2021**, 4, 36-45	36.5	88
625	Quantum mechanics based mechanisms for selective activation of hydrocarbons by mixed metal oxide heterogeneous catalysts A tribute to Robert Grasselli. *Catalysis Today*, **2021**, 363, 3-9	5.3	
624	Atomic and Molecular Unit Energy Conversion Catalysis of Carbon Dioxides in Value-Added Chemical Fuels. *Springer Series in Materials Science*, **2021**, 743-766	0.9	
623	Spatiotemporal Temperature and Pressure in Thermoplasmonic Gold Nanosphere-Water Systems. *ACS Nano*, **2021**, 15, 6276-6288	16.7	3
622	Reduction of N to Ammonia by Phosphate Molten Salt and Li Electrode: Proof of Concept Using Quantum Mechanics. *Journal of Physical Chemistry Letters*, **2021**, 12, 1696-1701	6.4	1
621	Hedgehog proteins create a dynamic cholesterol interface. *PLoS ONE*, **2021**, 16, e0246814	3.7	4
620	Operando Electrochemical Spectroscopy for CO on Cu(100) at pH 1 to 13: Validation of Grand Canonical Potential Predictions. *ACS Catalysis*, **2021**, 11, 3173-3181	13.1	3
619	Selective CO Electrochemical Reduction Enabled by a Tricomponent Copolymer Modifier on a Copper Surface. *Journal of the American Chemical Society*, **2021**, 143, 2857-2865	16.4	31
618	Diverse Phases of Carbonaceous Materials from Stochastic Simulations. *ACS Nano*, **2021**, 15, 6369-6385	16.7	2
617	Role of Ferryl Ion Intermediates in Fast Fenton Chemistry on Aqueous Microdroplets. *Environmental Science & Technology*, **2021**, 55, 14370-14377	10.3	5
616	Focus on the deformation mechanism at the interfacial layer in nano-reinforced polymers: A molecular dynamics study of silica - poly(methyl methacrylate) nano-composite. *Mechanics of Materials*, **2021**, 159, 103903	3.3	0
615	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
614	Development of the ReaxFF Reactive Force Field for Cu/Si Systems with Application to Copper Cluster Formation during Cu Diffusion Inside Silicon. *Journal of Physical Chemistry C*, **2021**, 125, 19455-19466	3.8	1
613	Entropic Stabilization of Water at Graphitic Interfaces. *Journal of Physical Chemistry Letters*, **2021**, 12, 9162-9168	6.4	0
612	Predicted Structure of Fully Activated Tas1R3/1R3' Homodimer Bound to G Protein and Natural Sugars: Structural Insights into G Protein Activation by a Class C Sweet Taste Homodimer with Natural Sugars. *Journal of the American Chemical Society*, **2021**, 143, 16824-16838	16.4	2
611	Graphitization of low-density amorphous carbon for electrocatalysis electrodes from ReaxFF reactive dynamics. *Carbon*, **2021**, 183, 940-947	10.4	4

610	The DFT-ReaxFF Hybrid Reactive Dynamics Method with Application to the Reductive Decomposition Reaction of the TFSI and DOL Electrolyte at a Lithium-Metal Anode Surface. *Journal of Physical Chemistry Letters*, **2021**, 12, 1300-1306	6.4	18
609	Use of Ligand Steric Properties to Control the Thermodynamics and Kinetics of Oxidative Addition and Reductive Elimination with Pincer-Ligated Rh Complexes. *Organometallics*, **2020**, 39, 1917-1933	3.8	5
608	Reaction mechanism and kinetics for CO reduction on nickel single atom catalysts from quantum mechanics. *Nature Communications*, **2020**, 11, 2256	17.4	59
607	Synergy between a Silver-Copper Surface Alloy Composition and Carbon Dioxide Adsorption and Activation. *ACS Applied Materials & Interfaces*, **2020**, 12, 25374-25382	9.5	7
606	Electrochemical Switching of a Fluorescent Molecular Rotor Embedded within a Bistable Rotaxane. *Journal of the American Chemical Society*, **2020**, 142, 11835-11846	16.4	19
605	Design of a Graphene Nitrene Two-Dimensional Catalyst Heterostructure Providing a Well-Defined Site Accommodating One to Three Metals, with Application to CO Reduction Electrocatalysis for the Two-Metal Case. *Journal of Physical Chemistry Letters*, **2020**, 11, 2541-2549	6.4	25
604	Effects of Surface Roughness on the Electrochemical Reduction of CO2 over Cu. *ACS Energy Letters*, **2020**, 5, 1206-1214	20.1	80
603	Highly Stable Organic Bisradicals Protected by Mechanical Bonds. *Journal of the American Chemical Society*, **2020**, 142, 7190-7197	16.4	10
602	Reaction Mechanism, Origins of Enantioselectivity, and Reactivity Trends in Asymmetric Allylic Alkylation: A Comprehensive Quantum Mechanics Investigation of a C(sp)-C(sp) Cross-Coupling. *Journal of the American Chemical Society*, **2020**, 142, 13917-13933	16.4	20
601	Group Vibrational Mode Assignments as a Broadly Applicable Tool for Characterizing Ionomer Membrane Structure as a Function of Degree of Hydration. *Chemistry of Materials*, **2020**, 32, 1828-1843	9.6	2
600	Synergetic Evolution of Sacrificial Bonds and Strain-Induced Defects Facilitating Large Deformation of the Bi2Te3 Semiconductor. *ACS Applied Energy Materials*, **2020**, 3, 3042-3048	6.1	2
599	Li-diffusion at the interface between Li-metal and [Pyr][TFSI]-ionic liquid: Ab initio molecular dynamics simulations. *Journal of Chemical Physics*, **2020**, 152, 031101	3.9	7
598	Si-Doped Fe Catalyst for Ammonia Synthesis at Dramatically Decreased Pressures and Temperatures. *Journal of the American Chemical Society*, **2020**, 142, 8223-8232	16.4	14
597	Atomistic Explanation of the Dramatically Improved Oxygen Reduction Reaction of Jagged Platinum Nanowires, 50 Times Better than Pt. *Journal of the American Chemical Society*, **2020**, 142, 8625-8632	16.4	32
596	Compressed Intermetallic PdCu for Enhanced Electrocatalysis. *ACS Energy Letters*, **2020**, 5, 3672-3680	20.1	19
595	Predicted Optimal Bifunctional Electrocatalysts for the Hydrogen Evolution Reaction and the Oxygen Evolution Reaction Using Chalcogenide Heterostructures Based on Machine Learning Analysis of in Silico Quantum Mechanics Based High Throughput Screening. *Journal of Physical Chemistry Letters*, **2020**, 11, 869-876	6.4	23
594	First-Order Phase Transition in Liquid Ag to the Heterogeneous G-Phase. *Journal of Physical Chemistry Letters*, **2020**, 11, 632-645	6.4	15
593	Tailoring a Three-Phase Microenvironment for High-Performance Oxygen Reduction Reaction in Proton Exchange Membrane Fuel Cells. *Matter*, **2020**, 3, 1774-1790	12.7	30

592	New Quantum Mechanics Based Methods for Multiscale Simulations with Applications to Reaction Mechanisms for Electrocatalysis. *Topics in Catalysis*, **2020**, 63, 1658-1666	2.3	1
591	Discovery of Dramatically Improved Ammonia Synthesis Catalysts through Hierarchical High-Throughput Catalyst Screening of the Fe(211) Surface. *Chemistry of Materials*, **2020**, 32, 9914-9924	9.6	3
590	Highly Selective Electrocatalytic Reduction of CO into Methane on Cu-Bi Nanoalloys. *Journal of Physical Chemistry Letters*, **2020**, 11, 7261-7266	6.4	20
589	Inertial dynamics of an interface with interfacial mass flux: Stability and flow fields□structure, inertial stabilization mechanism, degeneracy of Landau□ solution, effect of energy fluctuations, and chemistry-induced instabilities. *Physics of Fluids*, **2020**, 32, 082105	4.4	4
588	The Transition Metal Catalyzed [□s + □s + □s + □s] Pericyclic Reaction: Woodward-Hoffmann Rules, Aromaticity, and Electron Flow. *Journal of the American Chemical Society*, **2020**, 142, 19033-19039	16.4	4
587	Highly active and stable stepped Cu surface for enhanced electrochemical CO2 reduction to C2H4. *Nature Catalysis*, **2020**, 3, 804-812	36.5	118
586	Enhancing the Detonation Properties of Liquid Nitromethane by Adding Nitro-Rich Molecule Nitryl Cyanide. *Journal of Physical Chemistry C*, **2020**, 124, 9787-9794	3.8	4
585	CO Coupling Chemistry of a Terminal Mo Carbide: Sequential Addition of Proton, Hydride, and CO Releases Ethenone. *Journal of the American Chemical Society*, **2019**, 141, 15664-15674	16.4	20
584	Anomalies in Supercooled Water at ~230 K Arise from a 1D Polymer to 2D Network Topological Transformation. *Journal of Physical Chemistry Letters*, **2019**, 10, 6267-6273	6.4	7
583	Csp-Csp Bond-Forming Reductive Elimination from Well-Defined Copper(III) Complexes. *Journal of the American Chemical Society*, **2019**, 141, 3153-3159	16.4	56
582	Identifying Active Sites for CO Reduction on Dealloyed Gold Surfaces by Combining Machine Learning with Multiscale Simulations. *Journal of the American Chemical Society*, **2019**, 141, 11651-11657	16.4	59
581	Highly Efficient Ni-Doped Iron Catalyst for Ammonia Synthesis from Quantum-Mechanics-Based Hierarchical High-Throughput Catalyst Screening. *Journal of Physical Chemistry C*, **2019**, 123, 17375-17383	3.8	9
580	DFT Mechanistic Study of Methane Mono-Esterification by Hypervalent Iodine Alkane Oxidation Process. *Journal of Physical Chemistry C*, **2019**, 123, 15674-15684	3.8	9
579	Single-atom tailoring of platinum nanocatalysts for high-performance multifunctional electrocatalysis. *Nature Catalysis*, **2019**, 2, 495-503	36.5	258
578	Reaction mechanism and kinetics for ammonia synthesis on the Fe(211) reconstructed surface. *Physical Chemistry Chemical Physics*, **2019**, 21, 11444-11454	3.6	17
577	Effectively Increased Efficiency for Electroreduction of Carbon Monoxide Using Supported Polycrystalline Copper Powder Electrocatalysts. *ACS Catalysis*, **2019**, 9, 4709-4718	13.1	47
576	Dramatic differences in carbon dioxide adsorption and initial steps of reduction between silver and copper. *Nature Communications*, **2019**, 10, 1875	17.4	40
575	Initial Decomposition of HMX Energetic Material from Quantum Molecular Dynamics and the Molecular Structure Transition of □HMX to □HMX. *Journal of Physical Chemistry C*, **2019**, 123, 9231-9236	3.8	21

574	Reaction intermediates during operando electrocatalysis identified from full solvent quantum mechanics molecular dynamics. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 7718-7722	11.5	40
573	Electrocatalysis at Organic-Metal Interfaces: Identification of Structure-Reactivity Relationships for CO Reduction at Modified Cu Surfaces. *Journal of the American Chemical Society*, **2019**, 141, 7355-7364	16.4	76
572	Initial Steps in Forming the Electrode-Electrolyte Interface: HO Adsorption and Complex Formation on the Ag(111) Surface from Combining Quantum Mechanics Calculations and Ambient Pressure X-ray Photoelectron Spectroscopy. *Journal of the American Chemical Society*, **2019**, 141, 6946-6954	16.4	12
571	First principles-based multiscale atomistic methods for input into first principles nonequilibrium transport across interfaces. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 18193-18201	11.5	6
570	Formation of carbon-nitrogen bonds in carbon monoxide electrolysis. *Nature Chemistry*, **2019**, 11, 846-851	17.6	82
569	Interface Structure in Li-Metal/[Pyr][TFSI]-Ionic Liquid System from ab Initio Molecular Dynamics Simulations. *Journal of Physical Chemistry Letters*, **2019**, 10, 4577-4586	6.4	19
568	Computational and experimental demonstrations of one-pot tandem catalysis for electrochemical carbon dioxide reduction to methane. *Nature Communications*, **2019**, 10, 3340	17.4	81
567	Role of solvent-anion charge transfer in oxidative degradation of battery electrolytes. *Nature Communications*, **2019**, 10, 3360	17.4	26
566	Discovery of Novel Biased Opioid Receptor Ligands through Structure-Based Pharmacophore Virtual Screening and Experiment. *ChemMedChem*, **2019**, 14, 1783-1794	3.7	3
565	Accurate non-bonded potentials based on periodic quantum mechanics calculations for use in molecular simulations of materials and systems. *Journal of Chemical Physics*, **2019**, 151, 154111	3.9	16
564	Transport of hot carriers in plasmonic nanostructures. *Physical Review Materials*, **2019**, 3,	3.2	17
563	The PX Motif of DNA Binds Specifically to Escherichia coli DNA Polymerase I. *Biochemistry*, **2019**, 58, 575-581	3.2	4
562	Discrete Dimers of Redox-Active and Fluorescent Perylene Diimide-Based Rigid Isosceles Triangles in the Solid State. *Journal of the American Chemical Society*, **2019**, 141, 1290-1303	16.4	54
561	A Highly Active Star Decahedron Cu Nanocatalyst for Hydrocarbon Production at Low Overpotentials. *Advanced Materials*, **2019**, 31, e1805405	24	72
560	First-principles-based reaction kinetics from reactive molecular dynamics simulations: Application to hydrogen peroxide decomposition. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 18202-18208	11.5	18
559	Scalable Reactive Molecular Dynamics Simulations for Computational Synthesis. *Computing in Science and Engineering*, **2019**, 21, 64-75	1.5	3
558	Monolayer atomic crystal molecular superlattices. *Nature*, **2018**, 555, 231-236	50.4	220
557	Field-effect transistors made from solution-grown two-dimensional tellurene. *Nature Electronics*, **2018**, 1, 228-236	28.4	358

556	The 3D Structure of Human DP Prostaglandin G-Protein-Coupled Receptor Bound to Cyclopentanoindole Antagonist, Predicted Using the DuplexBiHelix Modification of the GEnSeMBLE Method. *Journal of Chemical Theory and Computation*, **2018**, 14, 1624-1642	6.4	6
555	Tellurium: Fast Electrical and Atomic Transport along the Weak Interaction Direction. *Journal of the American Chemical Society*, **2018**, 140, 550-553	16.4	81
554	Oxygen-Vacancy Abundant Ultrafine CoO/Graphene Composites for High-Rate Supercapacitor Electrodes. *Advanced Science*, **2018**, 5, 1700659	13.6	274
553	Predicted detonation properties at the Chapman-Jouguet state for proposed energetic materials (MTO and MTO3N) from combined ReaxFF and quantum mechanics reactive dynamics. *Physical Chemistry Chemical Physics*, **2018**, 20, 3953-3969	3.6	11
552	Defect-enriched iron fluoride-oxide nanoporous thin films bifunctional catalyst for water splitting. *Nature Communications*, **2018**, 9, 1809	17.4	137
551	Reaction Mechanism and Kinetics for Ammonia Synthesis on the Fe(111) Surface. *Journal of the American Chemical Society*, **2018**, 140, 6288-6297	16.4	78
550	Free Energy Landscape of Sodium Solvation into Graphite. *Journal of Physical Chemistry C*, **2018**, 122, 20064-20072	3.8	7
549	Electrochemical CO Reduction Builds Solvent Water into Oxygenate Products. *Journal of the American Chemical Society*, **2018**, 140, 9337-9340	16.4	95
548	In Silico Discovery of New Dopants for Fe-Doped Ni Oxyhydroxide (NiFe OOH) Catalysts for Oxygen Evolution Reaction. *Journal of the American Chemical Society*, **2018**, 140, 6745-6748	16.4	186
547	Extension of the Polarizable Charge Equilibration Model to Higher Oxidation States with Applications to Ge, As, Se, Br, Sn, Sb, Te, I, Pb, Bi, Po, and At Elements. *Journal of Physical Chemistry A*, **2018**, 122, 639-645	2.8	13
546	Identification of the Selective Sites for Electrochemical Reduction of CO to C2+ Products on Copper Nanoparticles by Combining Reactive Force Fields, Density Functional Theory, and Machine Learning. *ACS Energy Letters*, **2018**, 3, 2983-2988	20.1	48
545	Polarizable Charge Equilibration Model for Transition-Metal Elements. *Journal of Physical Chemistry A*, **2018**, 122, 9350-9358	2.8	7
544	QM-Mechanism-Based Hierarchical High-Throughput in Silico Screening Catalyst Design for Ammonia Synthesis. *Journal of the American Chemical Society*, **2018**, 140, 17702-17710	16.4	21
543	Reaction Mechanism for the Hydrogen Evolution Reaction on the Basal Plane Sulfur Vacancy Site of MoS Using Grand Canonical Potential Kinetics. *Journal of the American Chemical Society*, **2018**, 140, 16773-16782	16.4	56
542	The quantum mechanics-based polarizable force field for water simulations. *Journal of Chemical Physics*, **2018**, 149, 174502	3.9	23
541	Selective Extraction of C by a Tetragonal Prismatic Porphyrin Cage. *Journal of the American Chemical Society*, **2018**, 140, 13835-13842	16.4	64
540	Atomistic Description of Ionic Diffusion in PEO□iTFSI: Effect of Temperature, Molecular Weight, and Ionic Concentration. *Macromolecules*, **2018**, 51, 8987-8995	5.5	61
539	Synergy between Fe and Ni in the optimal performance of (Ni,Fe)OOH catalysts for the oxygen evolution reaction. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 5872-5877	11.5	237

538	Experimental and Ab Initio Ultrafast Carrier Dynamics in Plasmonic Nanoparticles. *Physical Review Letters*, **2017**, 118, 087401	7.4	83
537	Size-Matched Radical Multivalency. *Journal of the American Chemical Society*, **2017**, 139, 3986-3998	16.4	32
536	Full atomistic reaction mechanism with kinetics for CO reduction on Cu(100) from ab initio molecular dynamics free-energy calculations at 298 K. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 1795-1800	11.5	263
535	Nanotwins soften boron-rich boron carbide (B13C2). *Applied Physics Letters*, **2017**, 110, 111902	3.4	21
534	Probing the C–O Bond-Formation Step in Metalloporphyrin-Catalyzed C–H Oxygenation Reactions. *ACS Catalysis*, **2017**, 7, 4182-4188	13.1	37
533	Outstanding hydrogen evolution reaction catalyzed by porous nickel diselenide electrocatalysts. *Energy and Environmental Science*, **2017**, 10, 1487-1492	35.4	138
532	Subsurface oxide plays a critical role in CO activation by Cu(111) surfaces to form chemisorbed CO, the first step in reduction of CO. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 6706-6711	11.5	253
531	Polarizable charge equilibration model for predicting accurate electrostatic interactions in molecules and solids. *Journal of Chemical Physics*, **2017**, 146, 124117	3.9	34
530	Dual-Phase Mechanism for the Catalytic Conversion of n-Butane to Maleic Anhydride by the Vanadyl Pyrophosphate Heterogeneous Catalyst. *Journal of Physical Chemistry C*, **2017**, 121, 24069-24076	3.8	9
529	Ultrahigh Mass Activity for Carbon Dioxide Reduction Enabled by Gold-Iron Core-Shell Nanoparticles. *Journal of the American Chemical Society*, **2017**, 139, 15608-15611	16.4	151
528	The Oxygen Reduction Reaction on Graphene from Quantum Mechanics: Comparing Armchair and Zigzag Carbon Edges. *Journal of Physical Chemistry C*, **2017**, 121, 24408-24417	3.8	24
527	Role of Ligand Protonation in Dihydrogen Evolution from a Pentamethylcyclopentadienyl Rhodium Catalyst. *Inorganic Chemistry*, **2017**, 56, 11375-11386	5.1	29
526	The mechanism for catalytic hydrosilylation by bis(imino)pyridine iron olefin complexes supported by broken symmetry density functional theory. *Dalton Transactions*, **2017**, 46, 12507-12515	4.3	7
525	Nature of the Active Sites for CO Reduction on Copper Nanoparticles; Suggestions for Optimizing Performance. *Journal of the American Chemical Society*, **2017**, 139, 11642-11645	16.4	99
524	Predicting glycosaminoglycan surface protein interactions and implications for studying axonal growth. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 13697-13702	11.5	19
523	Multilayer Two-Dimensional Water Structure Confined in MoS2. *Journal of Physical Chemistry C*, **2017**, 121, 16021-16028	3.8	23
522	Computational Design of a Pincer Phosphinito Vanadium ((OPO)V) Propane Monoxygenation Homogeneous Catalyst Based on the Reduction-Coupled Oxo Activation (ROA) Mechanism. *ACS Catalysis*, **2017**, 7, 356-364	13.1	8
521	Quantum Mechanical Calculations of the Degradation in Perfluorinated Membranes Used in Fuel Cells **2017**, 241-269		

520	Schottky-Barrier-Free Contacts with Two-Dimensional Semiconductors by Surface-Engineered MXenes. *Journal of the American Chemical Society*, **2016**, 138, 15853-15856	16.4	278
519	Ab initio phonon coupling and optical response of hot electrons in plasmonic metals. *Physical Review B*, **2016**, 94,	3.3	89
518	Ultrafine jagged platinum nanowires enable ultrahigh mass activity for the oxygen reduction reaction. *Science*, **2016**, 354, 1414-1419	33.3	986
517	Nucleation of amorphous shear bands at nanotwins in boron suboxide. *Nature Communications*, **2016**, 7, 11001	17.4	30
516	Efficient hydrogen evolution by ternary molybdenum sulfoselenide particles on self-standing porous nickel diselenide foam. *Nature Communications*, **2016**, 7, 12765	17.4	248
515	Pressure-Dependent Polymorphism and Band-Gap Tuning of Methylammonium Lead Iodide Perovskite. *Angewandte Chemie - International Edition*, **2016**, 55, 6540-4	16.4	131
514	Pressure-Dependent Polymorphism and Band-Gap Tuning of Methylammonium Lead Iodide Perovskite. *Angewandte Chemie*, **2016**, 128, 6650-6654	3.6	11
513	Influence of Constitution and Charge on Radical Pairing Interactions in Tris-radical Tricationic Complexes. *Journal of the American Chemical Society*, **2016**, 138, 8288-300	16.4	23
512	Cubic Nonlinearity Driven Up-Conversion in High-Field Plasmonic Hot Carrier Systems. *Journal of Physical Chemistry C*, **2016**, 120, 21056-21062	3.8	16
511	Quantum Mechanical and Experimental Validation that Cyclobis(paraquat-p-phenylene) Forms a 1:1 Inclusion Complex with Tetrathiafulvalene. *Chemistry - A European Journal*, **2016**, 22, 2736-45	4.8	6
510	Prediction of the crystal packing of di-tetrazine-tetroxide (DTTO) energetic material. *Journal of Computational Chemistry*, **2016**, 37, 163-7	3.5	15
509	Suppression of surface recombination in CuInSe2 (CIS) thin films via Trioctylphosphine Sulfide (TOP:S) surface passivation. *Acta Materialia*, **2016**, 106, 171-181	8.4	12
508	Nonradiative Plasmon Decay and Hot Carrier Dynamics: Effects of Phonons, Surfaces, and Geometry. *ACS Nano*, **2016**, 10, 957-66	16.7	380
507	Homology modeling and molecular docking studies of Drosophila and Aedes sex peptide receptors. *Journal of Molecular Graphics and Modelling*, **2016**, 66, 115-22	2.8	5
506	Resolution of the Band Gap Prediction Problem for Materials Design. *Journal of Physical Chemistry Letters*, **2016**, 7, 1198-203	6.4	134
505	Prediction of the Chapman-Jouguet chemical equilibrium state in a detonation wave from first principles based reactive molecular dynamics. *Physical Chemistry Chemical Physics*, **2016**, 18, 2015-22	3.6	23
504	Structure-Based Sequence Alignment of the Transmembrane Domains of All Human GPCRs: Phylogenetic, Structural and Functional Implications. *PLoS Computational Biology*, **2016**, 12, e1004805	5	56
503	Sliding-Ring Catenanes. *Journal of the American Chemical Society*, **2016**, 138, 10214-25	16.4	29

502	Origin of low sodium capacity in graphite and generally weak substrate binding of Na and Mg among alkali and alkaline earth metals. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 3735-9	11.5	328
501	Oligorotaxane Radicals under Orders. *ACS Central Science*, **2016**, 2, 89-98	16.8	40
500	Redox Control of the Binding Modes of an Organic Receptor. *Journal of the American Chemical Society*, **2015**, 137, 11057-68	16.4	42
499	Theoretical and experimental studies of the dechlorination mechanism of carbon tetrachloride on a vivianite ferrous phosphate surface. *Journal of Physical Chemistry A*, **2015**, 119, 5714-22	2.8	12
498	The atomistic origin of the extraordinary oxygen reduction activity of PtNi fuel cell catalysts. *Chemical Science*, **2015**, 6, 3915-3925	9.4	47
497	The Reaction Mechanism with Free Energy Barriers for Electrochemical Dihydrogen Evolution on MoS2. *Journal of the American Chemical Society*, **2015**, 137, 6692-8	16.4	146
496	In Silico Design of Highly Selective Mo-V-Te-Nb-O Mixed Metal Oxide Catalysts for Ammoxidation and Oxidative Dehydrogenation of Propane and Ethane. *Journal of the American Chemical Society*, **2015**, 137, 13224-7	16.4	49
495	The charge-asymmetric nonlocally determined local-electric (CANDLE) solvation model. *Journal of Chemical Physics*, **2015**, 142, 064107	3.9	103
494	First principles-based multiparadigm, multiscale strategy for simulating complex materials processes with applications to amorphous SiC films. *Journal of Chemical Physics*, **2015**, 142, 174703	3.9	10
493	Accurate Ab Initio Quantum Mechanics Simulations of Bi2Se3 and Bi2Te3 Topological Insulator Surfaces. *Journal of Physical Chemistry Letters*, **2015**, 6, 3792-6	6.4	31
492	Fractal atomic-level percolation in metallic glasses. *Science*, **2015**, 349, 1306-10	33.3	93
491	Mechanisms and energetics of free radical initiated disulfide bond cleavage in model peptides and insulin by mass spectrometry. *Chemical Science*, **2015**, 6, 4550-4560	9.4	22
490	Free-Energy Barriers and Reaction Mechanisms for the Electrochemical Reduction of CO on the Cu(100) Surface, Including Multiple Layers of Explicit Solvent at pH 0. *Journal of Physical Chemistry Letters*, **2015**, 6, 4767-73	6.4	152
489	Folding of oligoviologens induced by radical-radical interactions. *Journal of the American Chemical Society*, **2015**, 137, 876-85	16.4	53
488	First-Principles Study of Iron Oxide Polytypes: Comparison of GGA+Uand Hybrid Functional Method. *Journal of Physical Chemistry C*, **2015**, 119, 556-562	3.8	18
487	Rhodium bis(quinolinyl)benzene complexes for methane activation and functionalization. *Chemistry - A European Journal*, **2015**, 21, 1286-93	4.8	23
486	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
485	Lithium Dendrite Inhibition on Post-Charge Anode Surface: The Kinetics Role. *Materials Research Society Symposia Proceedings*, **2015**, 1774, 31-39		

484	Atomistic Origin of Brittle Failure of Boron Carbide from Large-Scale Reactive Dynamics Simulations: Suggestions toward Improved Ductility. *Physical Review Letters*, **2015**, 115, 105501	7.4	76
483	Annealing kinetics of electrodeposited lithium dendrites. *Journal of Chemical Physics*, **2015**, 143, 134701	3.9	37
482	G protein-coupled odorant receptors: From sequence to structure. *Protein Science*, **2015**, 24, 1543-8	6.3	43
481	Electronic Structure of IrO2: The Role of the Metal d Orbitals. *Journal of Physical Chemistry C*, **2015**, 119, 11570-11577	3.8	54
480	Activation and Oxidation of Mesitylene C□H Bonds by (Phebox)Iridium(III) Complexes. *Organometallics*, **2015**, 34, 2879-2888	3.8	16
479	Mechanisms Underlying the Mpemba Effect in Water from Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2015**, 119, 2622-2629	3.8	22
478	DFT Study of Oxygen Reduction Reaction on Os/Pt Core□Shell Catalysts Validated by Electrochemical Experiment. *ACS Catalysis*, **2015**, 5, 1568-1580	13.1	63
477	Optimizing the oxygen evolution reaction for electrochemical water oxidation by tuning solvent properties. *Nanoscale*, **2015**, 7, 4514-21	7.7	19
476	Mechanism of O2 activation and methanol production by (di(2-pyridyl)methanesulfonate)Pt(II)Me(OH(n))((2-n)-) complex from theory with validation from experiment. *Journal of the American Chemical Society*, **2014**, 136, 2335-41	16.4	47
475	DFT Prediction of Oxygen Reduction Reaction on Palladium□Copper Alloy Surfaces. *ACS Catalysis*, **2014**, 4, 1189-1197	13.1	70
474	Dramatic increase in the oxygen reduction reaction for platinum cathodes from tuning the solvent dielectric constant. *Angewandte Chemie - International Edition*, **2014**, 53, 6669-72	16.4	27
473	Dealloyed Pt2Os nanoparticles for enhanced oxygen reduction reaction in acidic electrolytes. *Applied Catalysis B: Environmental*, **2014**, 150-151, 636-646	21.8	12
472	Design and validation of non-metal oxo complexes for C-H activation. *Chemical Communications*, **2014**, 50, 1748-50	5.8	15
471	ReaxFF Reactive Force-Field Modeling of the Triple-Phase Boundary in a Solid Oxide Fuel Cell. *Journal of Physical Chemistry Letters*, **2014**, 5, 4039-43	6.4	25
470	Dramatic Increase in the Oxygen Reduction Reaction for Platinum Cathodes from Tuning the Solvent Dielectric Constant. *Angewandte Chemie*, **2014**, 126, 6787-6790	3.6	6
469	DFT Virtual Screening Identifies Rhodium□Amidinate Complexes As Potential Homogeneous Catalysts for Methane-to-Methanol Oxidation. *ACS Catalysis*, **2014**, 4, 4455-4465	13.1	22
468	Predicted ligands for the human urotensin-II G protein-coupled receptor with some experimental validation. *ChemMedChem*, **2014**, 9, 1732-43	3.7	5
467	Inhibition of Hotspot Formation in Polymer Bonded Explosives Using an Interface Matching Low Density Polymer Coating at the Polymer□Explosive Interface. *Journal of Physical Chemistry C*, **2014**, 118, 19918-19928	3.8	18

466	Predicted 3D structures of olfactory receptors with details of odorant binding to OR1G1. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 1175-90	4.2	12
465	Interfacial thermodynamics of water and six other liquid solvents. *Journal of Physical Chemistry B*, **2014**, 118, 5943-56	3.4	27
464	Predicted roles of defects on band offsets and energetics at CIGS (Cu(In,Ga)Se2/CdS) solar cell interfaces and implications for improving performance. *Journal of Chemical Physics*, **2014**, 141, 094701	3.9	16
463	Deformation Induced Solid–Solid Phase Transitions in Gamma Boron. *Chemistry of Materials*, **2014**, 26, 4289-4298	9.6	8
462	The relation of mechanical properties and local structures in bulk Mg 54 (Cu 1−x Ag x) 35 Y 11 metallic glasses: Ab initio molecular dynamics simulations. *Computational Materials Science*, **2014**, 92, 313-317	3.2	6
461	General Multiobjective Force Field Optimization Framework, with Application to Reactive Force Fields for Silicon Carbide. *Journal of Chemical Theory and Computation*, **2014**, 10, 1426-39	6.4	81
460	ReaxFF reactive molecular dynamics on silicon pentaerythritol tetranitrate crystal validates the mechanism for the colossal sensitivity. *Physical Chemistry Chemical Physics*, **2014**, 16, 23779-91	3.6	19
459	Adaptive accelerated ReaxFF reactive dynamics with validation from simulating hydrogen combustion. *Journal of the American Chemical Society*, **2014**, 136, 9434-42	16.4	43
458	Decomposition of condensed phase energetic materials: interplay between uni- and bimolecular mechanisms. *Journal of the American Chemical Society*, **2014**, 136, 4192-200	16.4	104
457	Stability of NNO and NPO Nanotube Crystals. *Journal of Physical Chemistry Letters*, **2014**, 5, 485-9	6.4	5
456	Theoretical predictions for hot-carrier generation from surface plasmon decay. *Nature Communications*, **2014**, 5, 5788	17.4	475
455	Reactivity of a series of isostructural cobalt pincer complexes with CO2, CO, and H(+). *Inorganic Chemistry*, **2014**, 53, 13031-41	5.1	36
454	Nanocomposites of Tantalum-Based Pyrochlore and Indium Hydroxide Showing High and Stable Photocatalytic Activities for Overall Water Splitting and Carbon Dioxide Reduction. *Angewandte Chemie*, **2014**, 126, 14440-14444	3.6	3
453	Nanocomposites of tantalum-based pyrochlore and indium hydroxide showing high and stable photocatalytic activities for overall water splitting and carbon dioxide reduction. *Angewandte Chemie - International Edition*, **2014**, 53, 14216-20	16.4	22
452	Compressive Shear Reactive Molecular Dynamics Studies Indicating That Cocrystals of TNT/CL-20 Decrease Sensitivity. *Journal of Physical Chemistry C*, **2014**, 118, 30202-30208	3.8	51
451	Quantum chemical insights into the dissociation of nitric acid on the surface of aqueous electrolytes. *International Journal of Quantum Chemistry*, **2013**, 113, 413-417	2.1	11
450	Ex(2)Box: interdependent modes of binding in a two-nanometer-long synthetic receptor. *Journal of the American Chemical Society*, **2013**, 135, 12736-46	16.4	85
449	Computational modeling of structure and OH-anion diffusion in quaternary ammonium polysulfone hydroxide Polymer electrolyte for application in electrochemical devices. *Journal of Membrane Science*, **2013**, 431, 79-85	9.6	40

448	Scaled effective solvent method for predicting the equilibrium ensemble of structures with analysis of thermodynamic properties of amorphous polyethylene glycol-water mixtures. *Journal of Physical Chemistry B*, **2013**, 117, 916-27	3.4	12
447	Large-scale Molecular Simulations of Hypervelocity Impact of Materials. *Procedia Engineering*, **2013**, 58, 167-176		8
446	Equilibrium 2H/1H fractionation in organic molecules: III. Cyclic ketones and hydrocarbons. *Geochimica Et Cosmochimica Acta*, **2013**, 107, 82-95	5.5	16
445	Highly Shocked Polymer Bonded Explosives at a Nonplanar Interface: Hot-Spot Formation Leading to Detonation. *Journal of Physical Chemistry C*, **2013**, 117, 26551-26561	3.8	71
444	First-Principles-Based Reaction Kinetics for Decomposition of Hot, Dense Liquid TNT from ReaxFF Multiscale Reactive Dynamics Simulations. *Journal of Physical Chemistry C*, **2013**, 117, 21043-21054	3.8	57
443	A radically configurable six-state compound. *Science*, **2013**, 339, 429-33	33.3	140
442	Toward a lithium-"air" battery: the effect of CO2 on the chemistry of a lithium-oxygen cell. *Journal of the American Chemical Society*, **2013**, 135, 9733-42	16.4	262
441	Analytic Derivatives of Quartic-Scaling Doubly Hybrid XYGJ-OS Functional: Theory, Implementation, and Benchmark Comparison with M06-2X and MP2 Geometries for Nonbonded Compelexes. *Journal of Chemical Theory and Computation*, **2013**, 9, 1971-1976	6.4	12
440	Experimental and quantum mechanics investigations of early reactions of monomethylhydrazine with mixtures of NO2 and N2O4. *Combustion and Flame*, **2013**, 160, 970-981	5.3	22
439	The effect of different environments on Nafion degradation: Quantum mechanics study. *Journal of Membrane Science*, **2013**, 437, 276-285	9.6	14
438	Toward a Process-Based Molecular Model of SiC Membranes. 1. Development of a Reactive Force Field. *Journal of Physical Chemistry C*, **2013**, 117, 3308-3319	3.8	30
437	Relative unidirectional translation in an artificial molecular assembly fueled by light. *Journal of the American Chemical Society*, **2013**, 135, 18609-20	16.4	93
436	Formation of the -N(NO)N(NO)- polymer at high pressure and stabilization at ambient conditions. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 5321-5	11.5	10
435	The reaction mechanism of the enantioselective Tsuji allylation: inner-sphere and outer-sphere pathways, internal rearrangements, and asymmetric C-C bond formation. *Journal of the American Chemical Society*, **2012**, 134, 19050-60	16.4	89
434	Brønsted basicity of the air-water interface. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 18679-83	11.5	135
433	Predicted structure of agonist-bound glucagon-like peptide 1 receptor, a class B G protein-coupled receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 19988-93	11.5	41
432	Hydrophobic segregation, phase transitions and the anomalous thermodynamics of water/methanol mixtures. *Journal of Physical Chemistry B*, **2012**, 116, 13905-12	3.4	42
431	Anisotropic shock sensitivity for β-octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine energetic material under compressive-shear loading from ReaxFF-lg reactive dynamics simulations. *Journal of Applied Physics*, **2012**, 111, 124904	2.5	67

430	Chelating Base Effects in Palladium-Mediated Activation of Molecular Oxygen. *Organometallics*, **2012**, 31, 545-552	3.8	14
429	Deswelling Mechanisms of Surface-Grafted Poly(NIPAAm) Brush: Molecular Dynamics Simulation Approach. *Journal of Physical Chemistry C*, **2012**, 116, 15974-15985	3.8	27
428	Phosphofructokinase 1 glycosylation regulates cell growth and metabolism. *Science*, **2012**, 337, 975-80	33.3	389
427	Oxidative aliphatic C-H fluorination with fluoride ion catalyzed by a manganese porphyrin. *Science*, **2012**, 337, 1322-5	33.3	422
426	A Covalent Organic Framework that Exceeds the DOE 2015 Volumetric Target for H2 Uptake at 298 K. *Journal of Physical Chemistry Letters*, **2012**, 3, 2671-5	6.4	85
425	Structure prediction of G protein-coupled receptors and their ensemble of functionally important conformations. *Methods in Molecular Biology*, **2012**, 914, 237-54	1.4	22
424	How broadly tuned olfactory receptors equally recognize their agonists. Human OR1G1 as a test case. *Cellular and Molecular Life Sciences*, **2012**, 69, 4205-13	10.3	52
423	Development of a ReaxFF reactive force field for ettringite and study of its mechanical failure modes from reactive dynamics simulations. *Journal of Physical Chemistry A*, **2012**, 116, 3918-25	2.8	55
422	Reactive dynamics study of hypergolic bipropellants: monomethylhydrazine and dinitrogen tetroxide. *Journal of Physical Chemistry B*, **2012**, 116, 14136-45	3.4	16
421	DNA-linker-induced surface assembly of ultra dense parallel single walled carbon nanotube arrays. *Nano Letters*, **2012**, 12, 1129-35	11.5	44
420	Role of specific cations and water entropy on the stability of branched DNA motif structures. *Journal of Physical Chemistry B*, **2012**, 116, 12159-67	3.4	15
419	The para-substituent effect and pH-dependence of the organometallic Baeyer-Villiger oxidation of rhenium-carbon bonds. *Dalton Transactions*, **2012**, 41, 3758-63	4.3	9
418	The Role of Confined Water in Ionic Liquid Electrolytes for Dye-Sensitized Solar Cells. *Journal of Physical Chemistry Letters*, **2012**, 3, 556-9	6.4	28
417	Predicted Optimum Composition for the Glass-Forming Ability of Bulk Amorphous Alloys: Application to Cu-Zr-Al. *Journal of Physical Chemistry Letters*, **2012**, 3, 3143-8	6.4	29
416	High H2 uptake in Li-, Na-, K-metalated covalent organic frameworks and metal organic frameworks at 298 K. *Journal of Physical Chemistry A*, **2012**, 116, 1621-31	2.8	63
415	Anisotropic Shock Sensitivity of Cyclotrimethylene Trinitramine (RDX) from Compress-and-Shear Reactive Dynamics. *Journal of Physical Chemistry C*, **2012**, 116, 10198-10206	3.8	64
414	Bihelix: Towards de novo structure prediction of an ensemble of G-protein coupled receptor conformations. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 505-18	4.2	37
413	Solution-phase mechanistic study and solid-state structure of a tris(bipyridinium radical cation) inclusion complex. *Journal of the American Chemical Society*, **2012**, 134, 3061-72	16.4	112

412	Universal Correction of Density Functional Theory to Include London Dispersion (up to Lr, Element 103). *Journal of Physical Chemistry Letters*, **2012**, 3, 360-3	6.4	41
411	First-principles-based multiscale, multiparadigm molecular mechanics and dynamics methods for describing complex chemical processes. *Topics in Current Chemistry*, **2012**, 307, 1-42		8
410	Hypervelocity impact effect of molecules from Enceladus' plume and Titan's upper atmosphere on NASA's Cassini spectrometer from reactive dynamics simulation. *Physical Review Letters*, **2012**, 109, 213201	7.4	17
409	Anions dramatically enhance proton transfer through aqueous interfaces. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 10228-32	11.5	48
408	Synthesis of single-component metallic glasses by thermal spray of nanodroplets on amorphous substrates. *Applied Physics Letters*, **2012**, 100, 041909	3.4	17
407	Thermal decomposition of condensed-phase nitromethane from molecular dynamics from ReaxFF reactive dynamics. *Journal of Physical Chemistry B*, **2011**, 115, 6534-40	3.4	86
406	Thermodynamics of liquids: standard molar entropies and heat capacities of common solvents from 2PT molecular dynamics. *Physical Chemistry Chemical Physics*, **2011**, 13, 169-81	3.6	113
405	Accurate Band Gaps for Semiconductors from Density Functional Theory. *Journal of Physical Chemistry Letters*, **2011**, 2, 212-217	6.4	340
404	Thermodynamics of Water Stabilization of Carboxybetaine Hydrogels from Molecular Dynamics Simulations. *Journal of Physical Chemistry Letters*, **2011**, 2, 1757-1760	6.4	16
403	Oxygen Hydration Mechanism for the Oxygen Reduction Reaction at Pt and Pd Fuel Cell Catalysts. *Journal of Physical Chemistry Letters*, **2011**, 2, 572-576	6.4	98
402	Electronic--mechanical coupling in graphene from in situ nanoindentation experiments and multiscale atomistic simulations. *Nano Letters*, **2011**, 11, 1241-6	11.5	229
401	Development of a ReaxFF reactive force field for glycine and application to solvent effect and tautomerization. *Journal of Physical Chemistry B*, **2011**, 115, 249-61	3.4	150
400	Structure-based prediction of subtype selectivity of histamine H3 receptor selective antagonists in clinical trials. *Journal of Chemical Information and Modeling*, **2011**, 51, 3262-74	6.1	36
399	Development of interatomic ReaxFF potentials for Au-S-C-H systems. *Journal of Physical Chemistry A*, **2011**, 115, 10315-22	2.8	64
398	Phosphoramidite gold(I)-catalyzed diastereo- and enantioselective synthesis of 3,4-substituted pyrrolidines. *Journal of the American Chemical Society*, **2011**, 133, 5500-7	16.4	186
397	Elucidation of the dynamics for hot-spot initiation at nonuniform interfaces of highly shocked materials. *Physical Review B*, **2011**, 84,	3.3	78
396	ReaxFF-lg: correction of the ReaxFF reactive force field for London dispersion, with applications to the equations of state for energetic materials. *Journal of Physical Chemistry A*, **2011**, 115, 11016-22	2.8	278
395	Predicted structures and dynamics for agonists and antagonists bound to serotonin 5-HT2B and 5-HT2C receptors. *Journal of Chemical Information and Modeling*, **2011**, 51, 420-33	6.1	25

394	Interactions of poly(amidoamine) dendrimers with human serum albumin: binding constants and mechanisms. *ACS Nano*, **2011**, 5, 3456-68	16.7	87
393	Design of covalent organic frameworks for methane storage. *Journal of Physical Chemistry A*, **2011**, 115, 13852-7	2.8	76
392	Chemistry in the Center for Catalytic Hydrocarbon Functionalization: An Energy Frontier Research Center. *Catalysis Letters*, **2011**, 141, 213-221	2.8	33
391	Structures, Mechanisms, and Kinetics of Ammoxidation and Selective Oxidation of Propane Over the M2 Phase of MoVNbTeO Catalysts. *Topics in Catalysis*, **2011**, 54, 659-668	2.3	20
390	Predicted structures of agonist and antagonist bound complexes of adenosine A3 receptor. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 1878-97	4.2	27
389	Donor-acceptor oligorotaxanes made to order. *Chemistry - A European Journal*, **2011**, 17, 2107-19	4.8	49
388	Mechanism and kinetics for the initial steps of pyrolysis and combustion of 1,6-dicyclopropane-2,4-hexyne from ReaxFF reactive dynamics. *Journal of Physical Chemistry A*, **2011**, 115, 4941-50	2.8	81
387	Entropy and the driving force for the filling of carbon nanotubes with water. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 11794-8	11.5	251
386	Absolute Entropy and Energy of Carbon Dioxide Using the Two-Phase Thermodynamic Model. *Journal of Chemical Theory and Computation*, **2011**, 7, 1893-901	6.4	39
385	Surface and Electronic Properties of Hydrogen Terminated Si [001] Nanowires. *Journal of Physical Chemistry C*, **2011**, 115, 12586-12591	3.8	4
384	Hydroxylation Structure and Proton Transfer Reactivity at the Zinc Oxide□Water Interface. *Journal of Physical Chemistry C*, **2011**, 115, 8573-8579	3.8	72
383	Composition Dependence of Glass Forming Propensity in Al□Ni Alloys. *Journal of Physical Chemistry C*, **2011**, 115, 2320-2331	3.8	18
382	Electronic structures of Group 9 metallocorroles with axial ammines. *Inorganic Chemistry*, **2011**, 50, 764-70	4.1	17
381	Density-dependent liquid nitromethane decomposition: molecular dynamics simulations based on ReaxFF. *Journal of Physical Chemistry A*, **2011**, 115, 10181-202	2.8	95
380	Improved H2 Storage in Zeolitic Imidazolate Frameworks Using Li+, Na+, and K+ Dopants, with an Emphasis on Delivery H2 Uptake. *Journal of Physical Chemistry C*, **2011**, 115, 3507-3512	3.8	32
379	Measurement of the ground-state distributions in bistable mechanically interlocked molecules using slow scan rate cyclic voltammetry. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 20416-21	11.5	26
378	Elucidating glycosaminoglycan-protein-protein interactions using carbohydrate microarray and computational approaches. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 9747-52	11.5	82
377	A fast doubly hybrid density functional method close to chemical accuracy using a local opposite spin ansatz. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 19896-900	11.5	124

376	Thermodynamics of d-dimensional hard sphere fluids confined to micropores. *Journal of Chemical Physics*, **2011**, 134, 114502	3.9	9
375	Radically enhanced molecular recognition. *Nature Chemistry*, **2010**, 2, 42-9	17.6	247
374	Highly stable tetrathiafulvalene radical dimers in [3]catenanes. *Nature Chemistry*, **2010**, 2, 870-9	17.6	159
373	Self-assembly of carbon nanotubes into two-dimensional geometries using DNA origami templates. *Nature Nanotechnology*, **2010**, 5, 61-6	28.7	512
372	Direct atomistic simulation of brittle-to-ductile transition in silicon single crystals. *Materials Research Society Symposia Proceedings*, **2010**, 1272, 1		2
371	Generalized valence bond wave functions in quantum Monte Carlo. *Journal of Chemical Physics*, **2010**, 132, 164110	3.9	35
370	Experimental validation of the predicted binding site of Escherichia coli K1 outer membrane protein A to human brain microvascular endothelial cells: identification of critical mutations that prevent E. coli meningitis. *Journal of Biological Chemistry*, **2010**, 285, 37753-61	5.4	27
369	Quantum mechanics based force field for carbon (QMFF-Cx) validated to reproduce the mechanical and thermodynamics properties of graphite. *Journal of Chemical Physics*, **2010**, 133, 134114	3.9	16
368	Dearomatization reactions of N-heterocycles mediated by group 3 complexes. *Journal of the American Chemical Society*, **2010**, 132, 342-55	16.4	58
367	Application of the ReaxFF Reactive Force Field to Reactive Dynamics of Hydrocarbon Chemisorption and Decomposition. *Journal of Physical Chemistry C*, **2010**, 114, 5675-5685	3.8	118
366	Two-phase thermodynamic model for efficient and accurate absolute entropy of water from molecular dynamics simulations. *Journal of Physical Chemistry B*, **2010**, 114, 8191-8	3.4	218
365	First-Principles-Based Dispersion Augmented Density Functional Theory: From Molecules to Crystals. *Journal of Physical Chemistry Letters*, **2010**, 1, 2550-2555	6.4	36
364	Benzene C□H Bond Activation in Carboxylic Acids Catalyzed by O-Donor Iridium(III) Complexes: An Experimental and Density Functional Study. *Organometallics*, **2010**, 29, 742-756	3.8	48
363	Bimetallic reductive elimination from dinuclear Pd(III) complexes. *Journal of the American Chemical Society*, **2010**, 132, 14092-103	16.4	219
362	Unraveling Structural Models of Graphite Fluorides by Density Functional Theory Calculations. *Chemistry of Materials*, **2010**, 22, 2142-2154	9.6	51
361	Time resolved studies of interfacial reactions of ozone with pulmonary phospholipid surfactants using field induced droplet ionization mass spectrometry. *Journal of Physical Chemistry B*, **2010**, 114, 9496-503	3.4	30
360	Carbon□Oxygen Bond Forming Mechanisms in Rhenium Oxo-Alkyl Complexes. *Organometallics*, **2010**, 29, 2026-2033	3.8	9
359	Modeling High Rate Impact Sensitivity of Perfect RDX and HMX Crystals by ReaxFF Reactive Dynamics. *Journal of Energetic Materials*, **2010**, 28, 92-127	1.6	34

358	Physical mechanism of anisotropic sensitivity in pentaerythritol tetranitrate from compressive-shear reaction dynamics simulations. *Applied Physics Letters*, **2010**, 96, 081918	3.4	83
357	Development of a ReaxFF reactive force field for aqueous chloride and copper chloride. *Journal of Physical Chemistry A*, **2010**, 114, 3556-68	2.8	47
356	Competing, Coverage-Dependent Decomposition Pathways for C2Hy Species on Nickel (111). *Journal of Physical Chemistry C*, **2010**, 114, 20028-20041	3.8	33
355	Predicted 3D structures for adenosine receptors bound to ligands: comparison to the crystal structure. *Journal of Structural Biology*, **2010**, 170, 10-20	3.4	48
354	Theoretical Study of Solvent Effects on the Platinum-Catalyzed Oxygen Reduction Reaction. *Journal of Physical Chemistry Letters*, **2010**, 1, 856-861	6.4	172
353	Mechanically bonded macromolecules. *Chemical Society Reviews*, **2010**, 39, 17-29	58.5	380
352	Electrophilic, Ambiphilic, and Nucleophilic CH Bond Activation: Understanding the Electronic Continuum of CH Bond Activation Through Transition-State and Reaction Pathway Interaction Energy Decompositions. *Organometallics*, **2010**, 29, 6459-6472	3.8	86
351	Alkylgold complexes by the intramolecular aminoauration of unactivated alkenes. *Chemical Science*, **2010**, 1,	9.4	161
350	Zeolitic Imidazolate Frameworks as H2 Adsorbents: Ab Initio Based Grand Canonical Monte Carlo Simulation. *Journal of Physical Chemistry C*, **2010**, 114, 12039-12047	3.8	52
349	Molecular Dynamics Simulations of Metal Clusters Supported on Fishbone Carbon Nanofibers. *Journal of Physical Chemistry C*, **2010**, 114, 3522-3530	3.8	20
348	Development and Validation of ReaxFF Reactive Force Field for Hydrocarbon Chemistry Catalyzed by Nickel. *Journal of Physical Chemistry C*, **2010**, 114, 4939-4949	3.8	236
347	Definitive Band Gaps for Single-Wall Carbon Nanotubes. *Journal of Physical Chemistry Letters*, **2010**, 1, 2946-2950	6.4	149
346	Development and validation of a ReaxFF reactive force field for Cu cation/water interactions and copper metal/metal oxide/metal hydroxide condensed phases. *Journal of Physical Chemistry A*, **2010**, 114, 9507-14	2.8	140
345	Mechanism of C-F reductive elimination from palladium(IV) fluorides. *Journal of the American Chemical Society*, **2010**, 132, 3793-807	16.4	247
344	New surfactant classes for enhanced oil recovery and their tertiary oil recovery potential. *Journal of Petroleum Science and Engineering*, **2010**, 71, 23-29	4.4	222
343	Prediction of the three-dimensional structure for the rat urotensin II receptor, and comparison of the antagonist binding sites and binding selectivity between human and rat receptors from atomistic simulations. *ChemMedChem*, **2010**, 5, 1594-608	3.7	18
342	Water adsorption on stepped ZnO surfaces from MD simulation. *Surface Science*, **2010**, 604, 741-752	1.8	122
341	ReaxFF Monte Carlo reactive dynamics: Application to resolving the partial occupations of the M1 phase of the MoVNbTeO catalyst. *Catalysis Today*, **2010**, 157, 71-76	5.3	26

340	Doubly hybrid density functional for accurate descriptions of nonbond interactions, thermochemistry, and thermochemical kinetics. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 4963-8	11.5	280
339	Structure of polyamidoamide dendrimers up to limiting generations: a mesoscale description. *Journal of Chemical Physics*, **2009**, 130, 144902	3.9	42
338	Functionally rigid and degenerate molecular shuttles. *Chemistry - A European Journal*, **2009**, 15, 1115-22	4.8	41
337	The ReaxFF Monte Carlo reactive dynamics method for predicting atomistic structures of disordered ceramics: application to the Mo(3)VO(x) catalyst. *Angewandte Chemie - International Edition*, **2009**, 48, 7630-4	16.4	55
336	The optimum orbitals for the H2 + D?H + HD exchange reaction. *International Journal of Quantum Chemistry*, **2009**, 3, 63-66	2.1	3
335	The symmetric group and the spin generalized scf method. *International Journal of Quantum Chemistry*, **2009**, 4, 593-600	2.1	7
334	A bonding model for gold(I) carbene complexes. *Nature Chemistry*, **2009**, 1, 482-6	17.6	416
333	Alkyl polyglycoside surfactant□alcohol cosolvent formulations for improved oil recovery. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2009**, 339, 48-59	5.1	117
332	Cyclooctyne-based reagents for uncatalyzed click chemistry: A computational survey. *Organic and Biomolecular Chemistry*, **2009**, 7, 5255-8	3.9	53
331	On the impact of steric and electronic properties of ligands on gold(I)-catalyzed cycloaddition reactions. *Organic Letters*, **2009**, 11, 4798-801	6.2	146
330	Computational study of copper(II) complexation and hydrolysis in aqueous solutions using mixed cluster/continuum models. *Journal of Physical Chemistry A*, **2009**, 113, 9559-67	2.8	94
329	Partitioning of poly(amidoamine) dendrimers between n-octanol and water. *Environmental Science & Technology*, **2009**, 43, 5123-9	10.3	24
328	Product protection, the key to developing high performance methane selective oxidation catalysts. *Journal of the American Chemical Society*, **2009**, 131, 17110-5	16.4	100
327	Coupling of Raman radial breathing modes in double-wall carbon nanotubes and bundles of nanotubes. *Journal of Physical Chemistry B*, **2009**, 113, 7199-204	3.4	4
326	Reactions of group III biheterocyclic complexes. *Journal of the American Chemical Society*, **2009**, 131, 10269-78	16.4	51
325	Free energy barrier for molecular motions in bistable [2]rotaxane molecular electronic devices. *Journal of Physical Chemistry A*, **2009**, 113, 2136-43	2.8	38
324	Mechanism for activation of molecular oxygen by cis- and trans-(pyridine)2Pd(OAc)H: Pd(0) versus direct insertion. *Journal of the American Chemical Society*, **2009**, 131, 1416-25	16.4	36
323	Rigidity□Stability Relationship in Interlocked Model Complexes Containing Phenylene-Ethynylene-Based Disubstituted Naphthalene and Benzene. *Crystal Growth and Design*, **2009**, 9, 2300-2309	3.5	6

322	Sodium Diffusion through Aluminum-Doped Zeolite BEA System: Effect of Water Solvation. *Journal of Physical Chemistry C*, **2009**, 113, 819-826	3.8	7
321	Simulating the initial stage of phenolic resin carbonization via the ReaxFF reactive force field. *Journal of Physical Chemistry A*, **2009**, 113, 6891-4	2.8	85
320	Equilibrium 2H/1H fractionations in organic molecules: I. Experimental calibration of ab initio calculations. *Geochimica Et Cosmochimica Acta*, **2009**, 73, 7060-7075	5.5	35
319	Thermal decomposition process in algaenan of Botryococcus braunii race L. Part 2: Molecular dynamics simulations using the ReaxFF reactive force field. *Organic Geochemistry*, **2009**, 40, 416-427	3.1	82
318	Early maturation processes in coal. Part 2: Reactive dynamics simulations using the ReaxFF reactive force field on Morwell Brown coal structures. *Organic Geochemistry*, **2009**, 40, 1195-1209	3.1	134
317	Prediction of the size distributions of methanol-ethanol clusters detected in VUV laser/time-of-flight mass spectrometry. *Journal of Physical Chemistry A*, **2009**, 113, 6865-75	2.8	0
316	PAMAM dendrimers undergo pH responsive conformational changes without swelling. *Journal of the American Chemical Society*, **2009**, 131, 2798-9	16.4	222
315	Thermal decomposition of hydrazines from reactive dynamics using the ReaxFF reactive force field. *Journal of Physical Chemistry B*, **2009**, 113, 10770-8	3.4	76
314	Structures, Energetics, and Reaction Barriers for CHx Bound to the Nickel (111) Surface. *Journal of Physical Chemistry C*, **2009**, 113, 20290-20306	3.8	51
313	Recent advances on simulation and theory of hydrogen storage in metal-organic frameworks and covalent organic frameworks. *Chemical Society Reviews*, **2009**, 38, 1460-76	58.5	491
312	Initiation mechanisms and kinetics of pyrolysis and combustion of JP-10 hydrocarbon jet fuel. *Journal of Physical Chemistry A*, **2009**, 113, 1740-6	2.8	184
311	A push-button molecular switch. *Journal of the American Chemical Society*, **2009**, 131, 11571-80	16.4	105
310	Carbon cluster formation during thermal decomposition of octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine and 1,3,5-triamino-2,4,6-trinitrobenzene high explosives from ReaxFF reactive molecular dynamics simulations. *Journal of Physical Chemistry A*, **2009**, 113, 10619-40	2.8	189
309	First-principles investigation of anistropic hole mobilities in organic semiconductors. *Journal of Physical Chemistry B*, **2009**, 113, 8813-9	3.4	240
308	Parametrization of a reactive force field for aluminum hydride. *Journal of Chemical Physics*, **2009**, 131, 044501	3.9	31
307	Evaluation of B3LYP, X3LYP, and M06-Class Density Functionals for Predicting the Binding Energies of Neutral, Protonated, and Deprotonated Water Clusters. *Journal of Chemical Theory and Computation*, **2009**, 5, 1016-26	6.4	276
306	Temperature dependence of blue phosphorescent cyclometalated Ir(III) complexes. *Journal of the American Chemical Society*, **2009**, 131, 9813-22	16.4	482
305	Silicon nanowires as efficient thermoelectric materials. *Nature*, **2008**, 451, 168-71	50.4	2199

304	ReaxFF reactive force field for solid oxide fuel cell systems with application to oxygen ion transport in yttria-stabilized zirconia. *Journal of Physical Chemistry A*, **2008**, 112, 3133-40	2.8	77
303	Dendritic chelating agents. 2. U(VI) binding to poly(amidoamine) and poly(propyleneimine) dendrimers in aqueous solutions. *Environmental Science & Technology*, **2008**, 42, 1572-9	10.3	67
302	Covalent organic frameworks as exceptional hydrogen storage materials. *Journal of the American Chemical Society*, **2008**, 130, 11580-1	16.4	643
301	High H2 Storage of Hexagonal Metal Organic Frameworks from First-Principles-Based Grand Canonical Monte Carlo Simulations. *Journal of Physical Chemistry C*, **2008**, 112, 13431-13436	3.8	66
300	ReaxFF reactive force field for molecular dynamics simulations of hydrocarbon oxidation. *Journal of Physical Chemistry A*, **2008**, 112, 1040-53	2.8	1392
299	Experimentally-based recommendations of density functionals for predicting properties in mechanically interlocked molecules. *Journal of the American Chemical Society*, **2008**, 130, 14928-9	16.4	51
298	Lancifodilactone G: insights about an unusually stable enol. *Journal of Organic Chemistry*, **2008**, 73, 6853-62	4	16
297	Development and Application of a ReaxFF Reactive Force Field for Oxidative Dehydrogenation on Vanadium Oxide Catalysts. *Journal of Physical Chemistry C*, **2008**, 112, 14645-14654	3.8	106
296	ReaxFF reactive force field for the Y-doped BaZrO3 proton conductor with applications to diffusion rates for multigranular systems. *Journal of Physical Chemistry A*, **2008**, 112, 11414-22	2.8	79
295	Molecular dynamics simulations of the interactions between platinum clusters and carbon platelets. *Journal of Physical Chemistry A*, **2008**, 112, 1392-402	2.8	67
294	The predicted binding site and dynamics of peptide inhibitors to the Methuselah GPCR from Drosophila melanogaster. *Biochemistry*, **2008**, 47, 12740-9	3.2	4
293	Flat-Bottom Strategy for Improved Accuracy in Protein Side-Chain Placements. *Journal of Chemical Theory and Computation*, **2008**, 4, 2160-9	6.4	39
292	Reactive molecular dynamics force field for the dissociation of light hydrocarbons on Ni(111). *Molecular Simulation*, **2008**, 34, 967-972	2	10
291	Predictions of melting, crystallization, and local atomic arrangements of aluminum clusters using a reactive force field. *Journal of Chemical Physics*, **2008**, 129, 244506	3.9	43
290	De Novo Ultrascale Atomistic Simulations On High-End Parallel Supercomputers. *International Journal of High Performance Computing Applications*, **2008**, 22, 113-128	1.8	41
289	Modeling the sorption dynamics of NaH using a reactive force field. *Journal of Chemical Physics*, **2008**, 128, 164714	3.9	27
288	Structures, Mechanisms, and Kinetics of Selective Ammoxidation and Oxidation of Propane over Multi-metal Oxide Catalysts. *Topics in Catalysis*, **2008**, 50, 2-18	2.3	54
287	Characterization of the active site of yeast RNA polymerase II by DFT and ReaxFF calculations. *Theoretical Chemistry Accounts*, **2008**, 120, 479-489	1.9	36

286	Acid-catalyzed nucleophilic aromatic substitution: experimental and theoretical exploration of a multistep mechanism. *Chemistry - A European Journal*, **2008**, 14, 3954-60	4.8	23
285	The structure of human serotonin 2c G-protein-coupled receptor bound to agonists and antagonists. *Journal of Molecular Graphics and Modelling*, **2008**, 27, 66-81	2.8	29
284	Calculation of solvation free energies of charged solutes using mixed cluster/continuum models. *Journal of Physical Chemistry B*, **2008**, 112, 9709-19	3.4	459
283	Hydration of copper(II): new insights from density functional theory and the COSMO solvation model. *Journal of Physical Chemistry A*, **2008**, 112, 9104-12	2.8	84
282	Methylrhenium trioxide revisited: mechanisms for nonredox oxygen insertion in an M-CH3 bond. *Journal of the American Chemical Society*, **2007**, 129, 15794-804	16.4	45
281	Prediction of the 3D structure and dynamics of human DP G-protein coupled receptor bound to an agonist and an antagonist. *Journal of the American Chemical Society*, **2007**, 129, 10720-31	16.4	46
280	The inner-sphere process in the enantioselective Tsuji allylation reaction with (S)-t-Bu-phosphinooxazoline ligands. *Journal of the American Chemical Society*, **2007**, 129, 11876-7	16.4	117
279	Single-Site Vanadyl Activation, Functionalization, and Reoxidation Reaction Mechanism for Propane Oxidative Dehydrogenation on the Cubic V4O10 Cluster. *Journal of Physical Chemistry C*, **2007**, 111, 5115-5127	3.8	70
278	Pd-mediated activation of molecular oxygen: Pd(0) versus direct insertion. *Journal of the American Chemical Society*, **2007**, 129, 10361-9	16.4	49
277	Dendritic anion hosts: perchlorate uptake by G5-NH2 poly(propyleneimine) dendrimer in water and model electrolyte solutions. *Environmental Science & Technology*, **2007**, 41, 6521-7	10.3	40
276	Bifunctional anchors connecting carbon nanotubes to metal electrodes for improved nanoelectronics. *Journal of the American Chemical Society*, **2007**, 129, 9834-5	16.4	24
275	Methane Activation with Rhenium Catalysts. 1. Bidentate Oxygenated Ligands. *Organometallics*, **2007**, 26, 1505-1511	3.8	9
274	Lithium-doped metal-organic frameworks for reversible H2 storage at ambient temperature. *Journal of the American Chemical Society*, **2007**, 129, 8422-3	16.4	403
273	3-Dimensional structures of G protein-coupled receptors and binding sites of agonists and antagonists. *Journal of Nutrition*, **2007**, 137, 1528S-1538S; discussion 1548S	4.1	34
272	Prediction of the 3D structure of FMRF-amide neuropeptides bound to the mouse MrgC11 GPCR and experimental validation. *ChemBioChem*, **2007**, 8, 1527-39	3.8	21
271	Improved designs of metal-organic frameworks for hydrogen storage. *Angewandte Chemie - International Edition*, **2007**, 46, 6289-92	16.4	210
270	Prediction of the 3-D structure of rat MrgA G protein-coupled receptor and identification of its binding site. *Journal of Molecular Graphics and Modelling*, **2007**, 26, 800-12	2.8	13
269	Toward electrochemically controllable tristable three-station [2]catenanes. *Chemistry - an Asian Journal*, **2007**, 2, 76-93	4.5	65

268	Origin of static friction and its relationship to adhesion at the atomic scale. *Physical Review B*, **2007**, 75,	3.3	26
267	Threshold crack speed controls dynamical fracture of silicon single crystals. *Physical Review Letters*, **2007**, 99, 165502	7.4	106
266	Dynamic transition in the structure of an energetic crystal during chemical reactions at shock front prior to detonation. *Physical Review Letters*, **2007**, 99, 148303	7.4	113
265	Functional selectivity of dopamine D1 receptor agonists in regulating the fate of internalized receptors. *Neuropharmacology*, **2007**, 52, 562-75	5.5	38
264	A divide-and-conquer/cellular-decomposition framework for million-to-billion atom simulations of chemical reactions. *Computational Materials Science*, **2007**, 38, 642-652	3.2	82
263	Structures and Transport Properties of Hydrated Water-Soluble Dendrimer-Grafted Polymer Membranes for Application to Polymer Electrolyte Membrane Fuel Cells: Classical Molecular Dynamics Approach. *Journal of Physical Chemistry C*, **2007**, 111, 2759-2769	3.8	47
262	Metal□Organic Frameworks Provide Large Negative Thermal Expansion Behavior. *Journal of Physical Chemistry C*, **2007**, 111, 15185-15191	3.8	154
261	Mechanical and transport properties of the poly(ethylene oxide)-poly(acrylic acid) double network hydrogel from molecular dynamic simulations. *Journal of Physical Chemistry B*, **2007**, 111, 1729-37	3.4	121
260	pKa calculations of aliphatic amines, diamines, and aminoamides via density functional theory with a Poisson-Boltzmann continuum solvent model. *Journal of Physical Chemistry A*, **2007**, 111, 4422-30	2.8	115
259	The predicted 3D structures of the human M1 muscarinic acetylcholine receptor with agonist or antagonist bound. *ChemMedChem*, **2006**, 1, 878-90	3.7	30
258	Water formation on Pt and Pt-based alloys: a theoretical description of a catalytic reaction. *ChemPhysChem*, **2006**, 7, 992-1005	3.2	100
257	Threshold crack speed in dynamic fracture of silicon. *Materials Research Society Symposia Proceedings*, **2006**, 978,		3
256	Quantization of crack speeds in dynamic fracture of silicon: Multiparadigm ReaxFF modeling. *Materials Research Society Symposia Proceedings*, **2006**, 910, 7		
255	Predictions of CCR1 chemokine receptor structure and BX 471 antagonist binding followed by experimental validation. *Journal of Biological Chemistry*, **2006**, 281, 27613-20	5.4	78
254	Dynamic behavior of fully solvated beta2-adrenergic receptor, embedded in the membrane with bound agonist or antagonist. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 4882-7	11.5	41
253	The ferroelectric and cubic phases in BaTiO3 ferroelectrics are also antiferroelectric. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 14695-700	11.5	98
252	Molecular Modeling of Carbohydrates with No Charges, No Hydrogen Bonds, and No Atoms. *ACS Symposium Series*, **2006**, 271-284	0.4	4
251	Mechanism of the aerobic oxidation of alcohols by palladium complexes of N-heterocyclic carbenes. *Journal of the American Chemical Society*, **2006**, 128, 9651-60	16.4	71

250	Dynamics of the dissociation of hydrogen on stepped platinum surfaces using the ReaxFF reactive force field. *Journal of Physical Chemistry B*, **2006**, 110, 4274-82	3.4	110
249	Dynamic friction force in a carbon peapod oscillator. *Nanotechnology*, **2006**, 17, 5691-5695	3.4	43
248	Atomic-level simulations of seeman DNA nanostructures: the paranemic crossover in salt solution. *Biophysical Journal*, **2006**, 90, 1463-79	2.9	58
247	Fidelity of seryl-tRNA synthetase to binding of natural amino acids from HierDock first principles computations. *Protein Engineering, Design and Selection*, **2006**, 19, 195-203	1.9	10
246	Inaccessibility of beta-hydride elimination from -OH functional groups in Wacker-type oxidation. *Journal of the American Chemical Society*, **2006**, 128, 3132-3	16.4	59
245	Carboxylic solvents and O-donor ligand effects on CH activation by Pt(II). *Journal of the American Chemical Society*, **2006**, 128, 7404-5	16.4	67
244	Mechanistic Investigation of Iridium-Catalyzed Hydrovinylation of Olefins. *Organometallics*, **2006**, 25, 1618-1625	3.8	26
243	Mechanism of direct molecular oxygen insertion in a palladium(II)-hydride bond. *Inorganic Chemistry* , **2006**, 45, 9631-3	5.1	78
242	Solvent quality changes the structure of G8 PAMAM dendrimer, a disagreement with some experimental interpretations. *Journal of Physical Chemistry B*, **2006**, 110, 25628-32	3.4	81
241	Secondary organic aerosol formation by heterogeneous reactions of aldehydes and ketones: a quantum mechanical study. *Environmental Science & Technology*, **2006**, 40, 2333-8	10.3	34
240	Heterolytic CH Activation with a Cyclometalated Platinum(II) 6-Phenyl-4,4□di-tert-butyl-2,2-Bipyridine Complex. *Organometallics*, **2006**, 25, 4734-4737	3.8	47
239	Sulfation patterns of glycosaminoglycans encode molecular recognition and activity. *Nature Chemical Biology*, **2006**, 2, 467-73	11.7	417
238	Multiparadigm modeling of dynamical crack propagation in silicon using a reactive force field. *Physical Review Letters*, **2006**, 96, 095505	7.4	194
237	Alkylation of phenol: a mechanistic view. *Journal of Physical Chemistry A*, **2006**, 110, 2246-52	2.8	44
236	Mechanism of oxidative shuttling for [2]rotaxane in a Stoddart-Heath molecular switch: density functional theory study with continuum-solvation model. *Journal of Physical Chemistry B*, **2006**, 110, 7660-5	3.4	31
235	Development of the ReaxFF reactive force field for mechanistic studies of catalytic selective oxidation processes on BiMoO x. *Topics in Catalysis*, **2006**, 38, 93	2.3	89
234	Modeling the human PTC bitter-taste receptor interactions with bitter tastants. *Journal of Molecular Modeling*, **2006**, 12, 931-41	2	59
233	Effect of Solvent and pH on the Structure of PAMAM Dendrimers. *Macromolecules*, **2005**, 38, 979-991	5.5	354

232	Optimization and application of lithium parameters for the reactive force field, ReaxFF. *Journal of Physical Chemistry A*, **2005**, 109, 4575-82	2.8	79
231	A Perspective of Materials Modeling **2005**, 2707-2711		2
230	Density functional theory study of the geometry, energetics, and reconstruction process of Si111 surfaces. *Langmuir*, **2005**, 21, 12404-14	4	17
229	Nanophase segregation and water dynamics in the dendrion diblock copolymer formed from the Fr□het polyaryl ethereal dendrimer and linear PTFE. *Journal of Physical Chemistry B*, **2005**, 109, 10154-67	3.4	55
228	Intramolecular hydrogen bonding in disubstituted ethanes: general considerations and methodology in quantum mechanical calculations of the conformational equilibria of succinamate monoanion. *Journal of Physical Chemistry A*, **2005**, 109, 9083-8	2.8	7
227	Chemisorption of (CHx and C2Hy) hydrocarbons on Pt(111) clusters and surfaces from DFT studies. *Journal of Physical Chemistry B*, **2005**, 109, 297-311	3.4	62
226	ReaxFF(MgH) reactive force field for magnesium hydride systems. *Journal of Physical Chemistry A*, **2005**, 109, 851-9	2.8	209
225	The isomerization equilibrium between cis and trans chloride ruthenium olefin metathesis catalysts from quantum mechanics calculations. *Journal of the American Chemical Society*, **2005**, 127, 12218-9	16.4	94
224	Pd-mediated activation of molecular oxygen in a nonpolar medium. *Journal of the American Chemical Society*, **2005**, 127, 13172-9	16.4	91
223	The theoretical study on interaction of hydrogen with single-walled boron nitride nanotubes. I. The reactive force field ReaxFF(HBN) development. *Journal of Chemical Physics*, **2005**, 123, 114703	3.9	51
222	Test of the Binding Threshold Hypothesis for olfactory receptors: explanation of the differential binding of ketones to the mouse and human orthologs of olfactory receptor 912-93. *Protein Science* , **2005**, 14, 703-10	6.3	42
221	Molecular dynamics study of the binary Cu46Zr54 metallic glass motivated by experiments: Glass formation and atomic-level structure. *Physical Review B*, **2005**, 71,	3.3	199
220	Simulations on the thermal decomposition of a poly(dimethylsiloxane) polymer using the ReaxFF reactive force field. *Journal of the American Chemical Society*, **2005**, 127, 7192-202	16.4	316
219	Atomistic-scale simulations of the initial chemical events in the thermal initiation of triacetonetriperoxide. *Journal of the American Chemical Society*, **2005**, 127, 11053-62	16.4	136
218	Synthesis, structure, and reactivity of O-donor Ir(III) complexes: C-H activation studies with benzene. *Journal of the American Chemical Society*, **2005**, 127, 11372-89	16.4	68
217	Atomic simulations of kinetic friction and its velocity dependence at Al□Al and □Al2O3□Al2O3 interfaces. *Physical Review B*, **2005**, 72,	3.3	37
216	Thermal decomposition of RDX from reactive molecular dynamics. *Journal of Chemical Physics*, **2005** , 122, 54502	3.9	313
215	Mechanical properties of connected carbon nanorings via molecular dynamics simulation. *Physical Review B*, **2005**, 72,	3.3	54

214	Dynamics and thermodynamics of water in PAMAM dendrimers at subnanosecond time scales. *Journal of Physical Chemistry B*, **2005**, 109, 8663-72	3.4	120
213	Linear artificial molecular muscles. *Journal of the American Chemical Society*, **2005**, 127, 9745-59	16.4	617
212	Dendrimer enhanced ultrafiltration. 1. Recovery of Cu(II) from aqueous solutions using PAMAM dendrimers with ethylene diamine core and terminal NH2 groups. *Environmental Science & Technology*, **2005**, 39, 1366-77	10.3	243
211	Development of the ReaxFF reactive force field for describing transition metal catalyzed reactions, with application to the initial stages of the catalytic formation of carbon nanotubes. *Journal of Physical Chemistry A*, **2005**, 109, 493-9	2.8	332
210	The MPSim-Dock hierarchical docking algorithm: application to the eight trypsin inhibitor cocrystals. *Journal of Computational Chemistry*, **2005**, 26, 48-71	3.5	27
209	The Computational Materials Design Facility (CMDF): A powerful framework for multi-paradigm multi-scale simulations. *Materials Research Society Symposia Proceedings*, **2005**, 894, 1		2
208	Formation of water at a Pt(111) surface: A study using the reactive force field (ReaxFF). *Materials Research Society Symposia Proceedings*, **2005**, 900, 1		4
207	Theoretical study on interaction of hydrogen with single-walled boron nitride nanotubes. II. Collision, storage, and adsorption. *Journal of Chemical Physics*, **2005**, 123, 114704	3.9	41
206	Assessment of phenomenological models for viscosity of liquids based on nonequilibrium atomistic simulations of copper. *Journal of Chemical Physics*, **2005**, 123, 104506	3.9	24
205	Nanopores of carbon nanotubes as practical hydrogen storage media. *Applied Physics Letters*, **2005**, 87, 213113	3.4	29
204	Superprotonic phase transition of CsHSO4: A molecular dynamics simulation study. *Physical Review B*, **2005**, 72,	3.3	32
203	Aminomethanol water elimination: theoretical examination. *Journal of Chemical Physics*, **2005**, 123, 34304	3.9	25
202	Liquefaction of H2 molecules upon exterior surfaces of carbon nanotube bundles. *Applied Physics Letters*, **2005**, 86, 203108	3.4	26
201	Multi-paradigm multi-scale modeling of dynamical crack propagation in silicon using the ReaxFF reactive force field. *Materials Research Society Symposia Proceedings*, **2005**, 904, 1		
200	A Perspective of Materials Modeling **2005**, 2707-2711		
199	Selectivity and specificity of substrate binding in methionyl-tRNA synthetase. *Protein Science*, **2004**, 13, 2693-705	6.3	8
198	Design of a nanomechanical fluid control valve based on functionalized silicon cantilevers: coupling molecular mechanics with classical engineering design. *Nanotechnology*, **2004**, 15, 1405-1415	3.4	26
197	New alkali doped pillared carbon materials designed to achieve practical reversible hydrogen storage for transportation. *Physical Review Letters*, **2004**, 92, 166103	7.4	286

196	Adhesion and nonwetting-wetting transition in the Al/Al2O3 interface. *Physical Review B*, **2004**, 69,	3.3	158
195	The predicted 3D structure of the human D2 dopamine receptor and the binding site and binding affinities for agonists and antagonists. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 3815-20	11.5	134
194	Influence of Elastic Deformation on Single-Wall Carbon Nanotube Atomic Force Microscopy Probe Resolution. *Journal of Physical Chemistry B*, **2004**, 108, 13613-13618	3.4	34
193	Predicted 3D structure for the human beta 2 adrenergic receptor and its binding site for agonists and antagonists. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 2736-41	11.5	118
192	Making sense of olfaction through predictions of the 3-D structure and function of olfactory receptors. *Chemical Senses*, **2004**, 29, 269-90	4.8	69
191	Structure of PAMAM Dendrimers: Generations 1 through 11. *Macromolecules*, **2004**, 37, 6236-6254	5.5	408
190	Dendritic chelating agents. 1. Cu(II) binding to ethylene diamine core poly(amidoamine) dendrimers in aqueous solutions. *Langmuir*, **2004**, 20, 2640-51	4	187
189	From The Cover: The X3LYP extended density functional for accurate descriptions of nonbond interactions, spin states, and thermochemical properties. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 2673-7	11.5	782
188	Mechanism of homogeneous Ir(III) catalyzed regioselective arylation of olefins. *Journal of the American Chemical Society*, **2004**, 126, 352-63	16.4	172
187	Mechanistic analysis of hydroarylation catalysts. *Journal of the American Chemical Society*, **2004**, 126, 11658-65	16.4	138
186	HierVLS hierarchical docking protocol for virtual ligand screening of large-molecule databases. *Journal of Medicinal Chemistry*, **2004**, 47, 56-71	8.3	73
185	Nanophase-Segregation and Transport in Nafion 117 from Molecular Dynamics Simulations: Effect of Monomeric Sequence. *Journal of Physical Chemistry B*, **2004**, 108, 3149-3157	3.4	375
184	Thermodynamic Stability of Zimmerman Self-Assembled Dendritic Supramolecules from Atomistic Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2004**, 108, 10041-10052	3.4	11
183	Fluorinated imidazoles as proton carriers for water-free fuel cell membranes. *Journal of the American Chemical Society*, **2004**, 126, 15644-5	16.4	63
182	Adsorption of Atomic H and O on the (111) Surface of Pt3Ni Alloys. *Journal of Physical Chemistry B*, **2004**, 108, 8311-8323	3.4	65
181	Agostic interactions and dissociation in the first layer of water on Pt(111). *Journal of the American Chemical Society*, **2004**, 126, 9360-8	16.4	66
180	M3B: A Coarse Grain Force Field for Molecular Simulations of Malto-Oligosaccharides and Their Water Mixtures. *Journal of Physical Chemistry B*, **2004**, 108, 1414-1427	3.4	103
179	Predictions of Hole Mobilities in Oligoacene Organic Semiconductors from Quantum Mechanical Calculations *Journal of Physical Chemistry B*, **2004**, 108, 8614-8621	3.4	513

178	Accurate Energies and Structures for Large Water Clusters Using the X3LYP Hybrid Density Functional. *Journal of Physical Chemistry A*, **2004**, 108, 10518-10526	2.8	125
177	A Two-Stage Mechanism of Bimetallic Catalyzed Growth of Single-Walled Carbon Nanotubes. *Nano Letters*, **2004**, 4, 2331-2335	11.5	105
176	Molecular Dynamics Study of a Surfactant-Mediated Decane–Water Interface: Effect of Molecular Architecture of Alkyl Benzene Sulfonate. *Journal of Physical Chemistry B*, **2004**, 108, 12130-12140	3.4	187
175	The extended Perdew-Burke-Ernzerhof functional with improved accuracy for thermodynamic and electronic properties of molecular systems. *Journal of Chemical Physics*, **2004**, 121, 4068-82	3.9	130
174	Bonding Properties of the Water Dimer:´ A Comparative Study of Density Functional Theories. *Journal of Physical Chemistry A*, **2004**, 108, 2305-2313	2.8	163
173	First principles predictions of the structure and function of g-protein-coupled receptors: validation for bovine rhodopsin. *Biophysical Journal*, **2004**, 86, 1904-21	2.9	92
172	Interaction of E. coli outer-membrane protein A with sugars on the receptors of the brain microvascular endothelial cells. *Proteins: Structure, Function and Bioinformatics*, **2003**, 50, 213-21	4.2	30
171	Quantum Mechanical–Rapid Prototyping Applied to Methane Activation. *Topics in Catalysis*, **2003**, 23, 81-98	2.3	16
170	First principles calculations of the pKa values and tautomers of isoguanine and xanthine. *Chemical Research in Toxicology*, **2003**, 16, 1455-62	4	68
169	The structure–activity relationships of methane mono-oxygenase mimics in alkane activation. *Catalysis Today*, **2003**, 81, 263-286	5.3	10
168	The Source of Helicity in Perfluorinated N-Alkanes. *Macromolecules*, **2003**, 36, 5331-5341	5.5	97
167	A theoretical study of the conversion of gas phase methanediol to formaldehyde. *Journal of Chemical Physics*, **2003**, 119, 5117-5120	3.9	41
166	Shock waves in high-energy materials: the initial chemical events in nitramine RDX. *Physical Review Letters*, **2003**, 91, 098301	7.4	416
165	pKa Values of Guanine in Water: Density Functional Theory Calculations Combined with Poisson–Boltzmann Continuum–Solvation Model. *Journal of Physical Chemistry B*, **2003**, 107, 344-357	3.4	181
164	Fidelity of Phenylalanyl-tRNA Synthetase in Binding the Natural Amino Acids. *Journal of Physical Chemistry B*, **2003**, 107, 11549-11557	3.4	14
163	Structure, Bonding, and Stability of a Catalytica Platinum(II) Catalyst:´ A Computational Study. *Organometallics*, **2003**, 22, 2057-2068	3.8	66
162	Protein dynamics in a family of laboratory evolved thermophilic enzymes. *Journal of Molecular Biology*, **2003**, 327, 745-57	6.5	90
161	ReaxFFSiO Reactive Force Field for Silicon and Silicon Oxide Systems. *Journal of Physical Chemistry A*, **2003**, 107, 3803-3811	2.8	682

160	Criteria for formation of metallic glasses: The role of atomic size ratio. *Journal of Chemical Physics*, **2003**, 119, 9858-9870	3.9	74
159	The two-phase model for calculating thermodynamic properties of liquids from molecular dynamics: Validation for the phase diagram of Lennard-Jones fluids. *Journal of Chemical Physics*, **2003**, 119, 11792-11805	3.9	334
158	Quantum-mechanical calculations of the stabilities of fluxional isomers of C4H(7)(+) in solution. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 15-9	11.5	90
157	Cell multipole method for molecular simulations in bulk and confined systems. *Journal of Chemical Physics*, **2003**, 118, 5347-5355	3.9	11
156	Dynamic Charge Equilibration-Morse stretch force field: application to energetics of pure silica zeolites. *Journal of Computational Chemistry*, **2002**, 23, 1507-14	3.5	16
155	Conformational analysis of aqueous pullulan oligomers: an effective computational approach. *Polymer*, **2002**, 43, 509-516	3.9	14
154	Friction anisotropy at Ni(100)/(100) interfaces: Molecular dynamics studies. *Physical Review B*, **2002**, 66,	3.3	49
153	Peroxone chemistry: formation of H2O3 and ring-(HO2)(HO3) from O3/H2O2. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 15308-12	11.5	47
152	Prediction of structure and function of G protein-coupled receptors. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 12622-7	11.5	243
151	Structure-based design of mutant Methanococcus jannaschii tyrosyl-tRNA synthetase for incorporation of O-methyl-L-tyrosine. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 6579-84	11.5	20
150	Mechanism for antibody catalysis of the oxidation of water by singlet dioxygen. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 2636-41	11.5	66
149	The gas phase reaction of singlet dioxygen with water: a water-catalyzed mechanism. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 3376-81	11.5	69
148	An NMR and quantum-mechanical investigation of tetrahydrofuran solvent effects on the conformational equilibria of 1,4-butanedioic acid and its salts. *Journal of the American Chemical Society*, **2002**, 124, 4481-6	16.4	23
147	Computational insights on the challenges for polymerizing polar monomers. *Journal of the American Chemical Society*, **2002**, 124, 10198-210	16.4	77
146	The MSXX Force Field for the Barium Sulfate□Water Interface. *Journal of Physical Chemistry B*, **2002**, 106, 9951-9966	3.4	20
145	An NMR and quantum mechanical investigation of solvent effects on conformational equilibria of butanedinitrile. *Journal of the American Chemical Society*, **2002**, 124, 9318-22	16.4	17
144	First principles calculations of the tautomers and pK(a) values of 8-oxoguanine: implications for mutagenicity and repair. *Chemical Research in Toxicology*, **2002**, 15, 1023-35	4	100
143	Virtual screening for binding of phenylalanine analogues to phenylalanyl-tRNA synthetase. *Journal of the American Chemical Society*, **2002**, 124, 14442-9	16.4	27

142	Stability and Thermodynamics of the PtCl2 Type Catalyst for Activating Methane to Methanol: A Computational Study. *Organometallics*, **2002**, 21, 511-525	3.8	115
141	First principles multiscale modeling of physico-chemical aspects of tribology. *Tribology Series*, **2001**, 15-33		
140	Strategies for multiscale modeling and simulation of organic materials: polymers and biopolymers. *Computational and Theoretical Polymer Science*, **2001**, 11, 329-343		34
139	A multiscale approach for modeling crystalline solids. *Journal of Computer-Aided Materials Design*, **2001**, 8, 127-149		25
138	MPiSIM: Massively parallel simulation tool for metallic system. *Journal of Computer-Aided Materials Design*, **2001**, 8, 185-192		2
137	Kinks in the a/2<111> screw dislocation in Ta. *Journal of Computer-Aided Materials Design*, **2001**, 8, 117-125		6
136	Molecular dynamics simulations to compute the bulk response of amorphous PMMA. *Journal of Computer-Aided Materials Design*, **2001**, 8, 87-106		29
135	Crack propagation in a Tantalum nano-slab. *Journal of Computer-Aided Materials Design*, **2001**, 8, 151-159		6
134	Viscosities of liquid metal alloys from nonequilibrium molecular dynamics. *Journal of Computer-Aided Materials Design*, **2001**, 8, 233-243		71
133	A detailed model for the decomposition of nitramines: RDX and HMX. *Journal of Computer-Aided Materials Design*, **2001**, 8, 203-212		60
132	Application of lightweight threading techniques to computational chemistry. *Journal of Computer-Aided Materials Design*, **2001**, 8, 173-184		
131	Ab-initio studies of pressure induced phase transitions in BaO. *Journal of Computer-Aided Materials Design*, **2001**, 8, 193-202		16
130	Antibody catalysis of the oxidation of water. *Science*, **2001**, 293, 1806-11	33.3	226
129	Melting and crystallization in Ni nanoclusters: The mesoscale regime. *Journal of Chemical Physics*, **2001**, 115, 385-394	3.9	314
128	Critical behavior in spallation failure of metals. *Physical Review B*, **2001**, 63,	3.3	77
127	Atomistic Simulations of Corrosion Inhibitors Adsorbed on Calcite Surfaces I. Force field Parameters for Calcite. *Journal of Physical Chemistry B*, **2001**, 105, 10746-10752	3.4	36
126	ReaxFF: A Reactive Force Field for Hydrocarbons. *Journal of Physical Chemistry A*, **2001**, 105, 9396-9409	2.8	3390
125	Stabilization of coiled-coil peptide domains by introduction of trifluoroleucine. *Biochemistry*, **2001**, 40, 2790-6	3.2	146

124	Catalysis research of relevance to carbon management: progress, challenges, and opportunities. *Chemical Reviews*, **2001**, 101, 953-96	68.1	1188
123	Multiscale modeling and simulation methods with applications to dendritic polymers. *Computational and Theoretical Polymer Science*, **2001**, 11, 345-356		40
122	Antiferromagnetic band structure of La2CuO4: Becke-3□lee-Yang-Parr calculations. *Physical Review B*, **2001**, 63,	3.3	149
121	First Principles Calculation of pKa Values for 5-Substituted Uracils. *Journal of Physical Chemistry A*, **2001**, 105, 274-280	2.8	175
120	Chelators for radioimmunotherapy: I. NMR and ab initio calculation studies on 1,4,7,10-tetra(carboxyethyl)-1,4,7,10-tetraazacyclododecane (DO4Pr) and 1,4,7-tris(carboxymethyl)-10-(carboxyethyl)-1,4,7,10-tetraazacyclododecane (DO3A1Pr). *Inorganic Chemistry*, **2001**, 40, 4310-8	5.1	36
119	Molecular Dynamics Simulations of Supercooled Liquid Metals and Glasses. *Materials Research Society Symposia Proceedings*, **2000**, 644, 231		2
118	Conformation and proton configuration of pyrimidine deoxynucleoside oxidation damage products in water. *Chemical Research in Toxicology*, **2000**, 13, 462-70	4	59
117	Molecular modelling of dendrimers for nanoscale applications. *Nanotechnology*, **2000**, 11, 77-84	3.4	55
116	Thermal conductivity of carbon nanotubes. *Nanotechnology*, **2000**, 11, 65-69	3.4	844
115	Thermal conductivity of diamond and related materials from molecular dynamics simulations. *Journal of Chemical Physics*, **2000**, 113, 6888-6900	3.9	280
114	Thermochemistry for Hydrocarbon Intermediates Chemisorbed on Metal Surfaces: CHn-m(CH3)m with n = 1, 2, 3 and m□h on Pt, Ir, Os, Pd, Rh, and Ru. *Journal of the American Chemical Society*, **2000**, 122, 2309-2321	16.4	82
113	Stabilization of □-Helices by Dipole□Dipole Interactions within □-Helices. *Journal of Physical Chemistry B*, **2000**, 104, 7784-7789	3.4	37
112	Domain Motions in Phosphoglycerate Kinase using Hierarchical NEIMO Molecular Dynamics Simulations. *Journal of Physical Chemistry A*, **2000**, 104, 2375-2383	2.8	13
111	Solvent Effects on the Secondary Structures of Proteins. *Journal of Physical Chemistry A*, **2000**, 104, 2498-2503	2.8	18
110	The Mechanism for Unimolecular Decomposition of RDX (1,3,5-Trinitro-1,3,5-triazine), an ab Initio Study. *Journal of Physical Chemistry A*, **2000**, 104, 2261-2272	2.8	214
109	Application of the Self-Assembled Monolayer (SAM) Model to Dithiophosphate and Dithiocarbamate Engine Wear Inhibitors. *Journal of Physical Chemistry A*, **2000**, 104, 2508-2524	2.8	22
108	Morse Stretch Potential Charge Equilibrium Force Field for Ceramics: Application to the Quartz-Stishovite Phase Transition and to Silica Glass. *Physical Review Letters*, **1999**, 82, 1708-1711	7.4	154
107	Molecular-dynamics simulations of glass formation and crystallization in binary liquid metals: Cu-Ag and Cu-Ni. *Physical Review B*, **1999**, 59, 3527-3533	3.3	228

106	Studies of fullerenes and carbon nanotubes by an extended bond order potential. *Nanotechnology*, **1999**, 10, 263-268	3.4	33
105	Effects of Molecular Geometry on the STM Image Contrast of Methyl- and Bromo-Substituted Alkanes and Alkanols on Graphite. *Journal of Physical Chemistry B*, **1999**, 103, 9690-9699	3.4	43
104	Poly(amidoamine) Dendrimers: A New Class of High Capacity Chelating Agents for Cu(II) Ions. *Environmental Science & Technology*, **1999**, 33, 820-824	10.3	175
103	Strain Rate Induced Amorphization in Metallic Nanowires. *Physical Review Letters*, **1999**, 82, 2900-2903	7.4	246
102	Ab Initio Quantum Mechanical Study of the Structures and Energies for the Pseudorotation of 5-Dehydroxy Analogues of 2-Deoxyribose and Ribose Sugars. *Journal of the American Chemical Society*, **1999**, 121, 985-993	16.4	71
101	Oxidation of Methanol on 2nd and 3rd Row Group VIII Transition Metals (Pt, Ir, Os, Pd, Rh, and Ru): Application to Direct Methanol Fuel Cells. *Journal of the American Chemical Society*, **1999**, 121, 10928-10941	16.4	370
100	Mechanism and Energetics for Complexation of90Y with 1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraacetic Acid (DOTA), a Model for Cancer Radioimmunotherapy. *Journal of the American Chemical Society*, **1999**, 121, 6142-6151	16.4	65
99	Tunneling Mechanism Implications from an STM Study of H3C(CH2)15HCCCH(CH2)15CH3 on Graphite and C14H29OH on MoS2. *Journal of Physical Chemistry B*, **1999**, 103, 7077-7080	3.4	22
98	Efficient Monte Carlo method for free energy evaluation of polymer chains. *Fluid Phase Equilibria*, **1998**, 144, 415-425	2.5	19
97	Chemisorption of Organics on Platinum. 1. The Interstitial Electron Model. *Journal of Physical Chemistry B*, **1998**, 102, 9481-9491	3.4	65
96	Correlation Analysis of Chemical Bonds. *Journal of Physical Chemistry A*, **1998**, 102, 2919-2933	2.8	35
95	Substrate assistance in the mechanism of family 18 chitinases: theoretical studies of potential intermediates and inhibitors. *Journal of Molecular Biology*, **1998**, 280, 913-23	6.5	99
94	Chemisorption of Organics on Platinum. 2. Chemisorption of C2Hx and CHx on Pt(111). *Journal of Physical Chemistry B*, **1998**, 102, 9492-9500	3.4	94
93	Energetics, structure, mechanical and vibrational properties of single-walled carbon nanotubes. *Nanotechnology*, **1998**, 9, 184-191	3.4	411
92	Calculation of Mechanical, Thermodynamic and Transport Properties of Metallic Glass Formers. *Materials Research Society Symposia Proceedings*, **1998**, 554, 43		101
91	Position of K Atoms in Doped Single-Walled Carbon Nanotube Crystals. *Physical Review Letters*, **1998**, 80, 5556-5559	7.4	110
90	Recent Advances in Simulation of Dendritic Polymers. *Materials Research Society Symposia Proceedings*, **1998**, 543, 299		2
89	Conduction properties of the organic superconductor (BEDT-TTF)2Cu(NCS)2 based on Hubbard-Unrestricted-Hartree-Fock band calculations. *Physical Review B*, **1997**, 56, 11907-11919	3.3	25

88	Dynamics of Bengal Rose Encapsulated in the Meijer Dendrimer Box. *Journal of the American Chemical Society*, **1997**, 119, 7458-7462	16.4	83
87	Theoretical Description of the STM Images of Alkanes and Substituted Alkanes Adsorbed on Graphite. *Journal of Physical Chemistry B*, **1997**, 101, 5996-6020	3.4	71
86	Distance Dependent Hydrogen Bond Potentials for Nucleic Acid Base Pairs from ab Initio Quantum Mechanical Calculations (LMP2/cc-pVTZ). *Journal of Physical Chemistry B*, **1997**, 101, 4851-4859	3.4	92
85	Source of Image Contrast in STM Images of Functionalized Alkanes on Graphite: A Systematic Functional Group Approach. *Journal of Physical Chemistry B*, **1997**, 101, 5978-5995	3.4	249
84	Molecular dynamics for very large systems on massively parallel computers: The MPSim program. *Journal of Computational Chemistry*, **1997**, 18, 501-521	3.5	74
83	Constant Temperature Constrained Molecular Dynamics: The NewtonEuler Inverse Mass Operator Method. *The Journal of Physical Chemistry*, **1996**, 100, 10508-10517		64
82	Self-Assembled Monolayer Mechanism for Corrosion Inhibition of Iron by Imidazolines. *Langmuir*, **1996**, 12, 6419-6428	4	190
81	Band structures of II-VI semiconductors using Gaussian basis functions with separable ab initio pseudopotentials: Application to prediction of band offsets. *Physical Review B*, **1996**, 53, 1377-1387	3.3	36
80	Dual-space approach for density-functional calculations of two- and three-dimensional crystals using Gaussian basis functions. *Physical Review B*, **1995**, 52, 2348-2361	3.3	33
79	Ab initio predictions of large hyperpolarizability push-pull polymers. Julolidinyl-n-isoxazolone and julolidinyl-n-N,N?-diethylthiobarbituric acid. *Chemical Physics Letters*, **1995**, 242, 543-547	2.5	14
78	A generalized direct inversion in the iterative subspace approach for generalized valence bond wave functions. *Journal of Chemical Physics*, **1994**, 100, 1226-1235	3.9	24
77	Protein simulations using techniques suitable for very large systems: the cell multipole method for nonbond interactions and the Newton-Euler inverse mass operator method for internal coordinate dynamics. *Proteins: Structure, Function and Bioinformatics*, **1994**, 20, 227-47	4.2	77
76	Accurate First Principles Calculation of Molecular Charge Distributions and Solvation Energies from Ab Initio Quantum Mechanics and Continuum Dielectric Theory. *Journal of the American Chemical Society*, **1994**, 116, 11875-11882	16.4	953
75	New pseudospectral algorithms for electronic structure calculations: Length scale separation and analytical two-electron integral corrections. *Journal of Chemical Physics*, **1994**, 101, 4028-4041	3.9	117
74	Energetics of Third-Row Transition Metal Methylidene Ions MCH2+ (M = La, Hf, Ta, W, Re, Os, Ir, Pt, Au). *Journal of the American Chemical Society*, **1994**, 116, 8733-8740	16.4	104
73	Electron-phonon interactions and superconductivity in K3C60. *Physical Review B*, **1993**, 48, 13959-13970	3.3	48
72	Atomic level simulations on a million particles: The cell multipole method for Coulomb and London nonbond interactions. *Journal of Chemical Physics*, **1992**, 97, 4309-4315	3.9	366
71	Optimal spline cutoffs for Coulomb and van der Waals interactions. *Chemical Physics Letters*, **1992**, 193, 197-201	2.5	22

70	Prediction of fullerene packing in C60 and C70 crystals. *Nature*, **1991**, 351, 464-467	50.4	292
69	Mechanical properties and force field parameters for polyethylene crystal. *The Journal of Physical Chemistry*, **1991**, 95, 2260-2272		140
68	Charge equilibration for molecular dynamics simulations. *The Journal of Physical Chemistry*, **1991**, 95, 3358-3363		2479
67	DREIDING: a generic force field for molecular simulations. *The Journal of Physical Chemistry*, **1990**, 94, 8897-8909		4645
66	Starburst Dendrimers: Molecular-Level Control of Size, Shape, Surface Chemistry, Topology, and Flexibility from Atoms to Macroscopic Matter. *Angewandte Chemie International Edition in English*, **1990**, 29, 138-175		2705
65	Starburst-Dendrimere: Kontrolle von Größe, Gestalt, Oberflächenchemie, Topologie und Flexibilität beim Übergang von Atomen zu makroskopischer Materie. *Angewandte Chemie*, **1990**, 102, 119-157	3.6	387
64	Singlet–triplet energy gaps in fluorine-substituted methylenes and silylenes. *Journal of Chemical Physics*, **1990**, 93, 4986-4993	3.9	38
63	Acceleration of convergence for lattice sums. *The Journal of Physical Chemistry*, **1989**, 93, 7320-7327		364
62	Starburst dendrimers. 5. Molecular shape control. *Journal of the American Chemical Society*, **1989**, 111, 2339-2341	16.4	447
61	Charge density waves, spin density waves, and Peierls distortions in one-dimensional metals. I. Hartree–Fock studies of Cu, Ag, Au, Li, and Na. *Journal of Chemical Physics*, **1988**, 88, 277-302	3.9	43
60	Correlation-consistent configuration interaction: Accurate bond dissociation energies from simple wave functions. *Journal of Chemical Physics*, **1988**, 88, 3132-3140	3.9	89
59	Theoretical studies of oxidative addition and reductive elimination. 2. Reductive coupling of hydrogen-hydrogen, hydrogen-carbon, and carbon-carbon bonds from palladium and platinum complexes. *Organometallics*, **1986**, 5, 609-622	3.8	209
58	New concepts of metallic bonding based on valence-bond ideas. *Physical Review Letters*, **1985**, 55, 2563-2566	7.4	100
57	New concepts of bonding in nonperiodic metallic systems. *Journal of Non-Crystalline Solids*, **1985**, 75, 149-159	3.9	27
56	Modified generalized valence-bond method: A simple correction for the electron correlation missing in generalized valence-bond wave functions; Prediction of double-well states for Cr2 and Mo2. *Physical Review Letters*, **1985**, 54, 661-664	7.4	117
55	The lower electronic states of MoN. *Chemical Physics*, **1983**, 81, 263-271	2.3	21
54	Olefin metathesis - a mechanistic study of high-valent Group VI catalysts. *Journal of the American Chemical Society*, **1982**, 104, 448-456	16.4	203
53	Theoretical studies of oxygen binding. *Annals of the New York Academy of Sciences*, **1981**, 367, 419-33	6.5	8

52	Flexible d basis sets for scandium through copper. *The Journal of Physical Chemistry*, **1981**, 85, 2607-2611		130
51	The Rydberg states of trans-butadiene from generalized valence bond and configuration interaction calculations. *Chemical Physics*, **1980**, 53, 251-263	2.3	35
50	The Rydberg states of trans-1,3-5-hexatriene from ab initio and configuration interaction calculations. *Chemical Physics*, **1980**, 53, 265-277	2.3	11
49	Ab initio studies of the x-ray absorption edge in copper complexes. I. Atomic Cu2+ and Cu(ii)Cl2. *Physical Review B*, **1980**, 22, 2767-2776	3.3	224
48	Theoretical studies of the dissociative adsorption of H2 on Ni(001) using ab initio parameterized LEPS calculations. *Surface Science*, **1980**, 95, 391-402	1.8	32
47	THEORETICAL STUDIES OF THE BONDING OF O2 TO HEMOGLOBIN; IMPLICATIONS FOR COOPERATIVITY **1979**, 87-123		4
46	SINGLET MOLECULAR OXYGEN CHEMISTRY AND IMPLICATIONS FOR FLAVIN-COFACTOR HYDROXYLATIONS **1979**, 513-555		1
45	The excited electronic states of all-trans-1,3,5-hexatriene. *Chemical Physics Letters*, **1979**, 60, 197-200	2.5	25
44	Electronic states of silicon vacancy. I. Covalent states. *Physical Review B*, **1978**, 18, 2831-2839	3.3	36
43	Ab initio effective potentials for silicon. *Physical Review B*, **1977**, 15, 5038-5048	3.3	70
42	Theoretical studies of the oxidized and reduced states of a model for the active site of rubredoxin. *Journal of the American Chemical Society*, **1977**, 99, 3505-7	16.4	15
41	Ab initio theoretical results on the stability of cyclic ozone. *Journal of Chemical Physics*, **1977**, 67, 2377	3.9	39
40	Theoretical studies of the geometries of O and S overlayers on the (100) surface of nickel. *Solid State Communications*, **1977**, 23, 907-910	1.6	13
39	The low lying states of ammonia; generalized valence bond and configuration interaction studies. *Chemical Physics*, **1977**, 19, 131-136	2.3	41
38	The Self-Consistent Field Equations for Generalized Valence Bond and Open-Shell HartreeFock Wave Functions **1977**, 79-127		173
37	The low-lying excited states of water, methanol, and dimethyl ether. *Chemical Physics*, **1976**, 18, 1-11	2.3	42
36	Dipole moments and electric field gradients for correlated wavefunctions of NO: The X 2 , A 2 , and D 2 states. *Chemical Physics Letters*, **1975**, 33, 18-24	2.5	24
35	Spatially projected generalized valence bond description of the pi-states of allyl radical. *Theoretica Chimica Acta*, **1975**, 37, 253-267		10

34	Nature of the excited states of He2. *Physical Review A*, **1975**, 12, 1203-1221	2.6	97
33	Configuration interaction studies of O3 and O+3. Ground and excited states. *Journal of Chemical Physics*, **1975**, 62, 3912-3924	3.9	206
32	The orbital description of the potential energy curves and properties of the lower excited states of the BH molecule. *Chemical Physics*, **1974**, 3, 297-316	2.3	36
31	Theoretical evidence for bound electronic excited states of ozone. *Chemical Physics Letters*, **1973**, 23, 457-462	2.5	60
30	Generalized valence bond description of bonding in low-lying states of molecules. *Accounts of Chemical Research*, **1973**, 6, 368-376	24.3	427
29	Orbital Description and Properties of the BH Molecule. *Journal of Chemical Physics*, **1972**, 57, 5296-5310	3.9	16
28	Orbital Description of the Excited States of LiH. *Journal of Chemical Physics*, **1972**, 56, 3348-3359	3.9	14
27	Ab Initio Effective Potentials for Use in Molecular Calculations. *Journal of Chemical Physics*, **1972**, 56, 2685-2701	3.9	121
26	The valence bond Aufbau principle for molecular excited states. *Chemical Physics Letters*, **1972**, 16, 157-163	2.5	7
25	The role of kinetic energy in chemical binding. *Theoretica Chimica Acta*, **1972**, 26, 195-210		77
24	The incorporation of quadratic convergence into open-shell self-consistent field equations. *Chemical Physics Letters*, **1970**, 6, 147-151	2.5	48
23	Exchange kinetic energy, contragradience, and chemical binding. *Chemical Physics Letters*, **1970**, 5, 45-49	2.5	39
22	Spin-Generalized SCF Wavefunctions for H2O, OH, and O. *Journal of Chemical Physics*, **1970**, 53, 1803-1814	3.9	20
21	Core Polarization and Hyperfine Structure of the B, C, N, O, and F Atoms. *Physical Review*, **1969**, 182, 48-64		63
20	New Approach to Energy-Band Calculations with Results for Lithium Metal. *Physical Review Letters*, **1969**, 23, 300-303	7.4	28
19	Electronic Structure of LiH According to a Generalization of the Valence-Bond Method. *Journal of Chemical Physics*, **1969**, 50, 4524-4532	3.9	47
18	Improved Quantum Theory of Many-Electron Systems. V. The Spin-Coupling Optimized GI Method. *Journal of Chemical Physics*, **1969**, 51, 1073-1087	3.9	186
17	Excited States of H2O using improved virtual orbitals. *Chemical Physics Letters*, **1969**, 3, 414-418	2.5	546

16	Ab Initio Calculations on the H2+D2=2HD Four-Center Exchange Reaction. I. Elements of the Reaction Surface. *Journal of Chemical Physics*, **1969**, 51, 716-731	3.9	66
15	New Foundation for the Use of Pseudopotentials in Metals. *Physical Review*, **1968**, 174, 659-662		87
14	New Type of Wave Function for Li, Be+, and B++. *Physical Review*, **1968**, 169, 120-130		55
13	Wavefunctions and Correlation Energies for Two-, Three-, and Four-Electron Atoms. *Journal of Chemical Physics*, **1968**, 48, 1008-1017	3.9	58
12	Concerning the Stability of the Negative Ions H□and Li□*Physical Review*, **1968**, 172, 7-12		24
11	Magnetic Hyperfine Structure and Core Polarization in the Excited States of Lithium. *Physical Review*, **1968**, 176, 106-114		33
10	Improved Quantum Theory of Many-Electron Systems. III. The GF Method. *Journal of Chemical Physics*, **1968**, 48, 450-461	3.9	93
9	Improved Quantum Theory of Many-Electron Systems. IV. Properties of GF Wavefunctions. *Journal of Chemical Physics*, **1968**, 48, 5337-5347	3.9	37
8	Magnetic Hyperfine Structure of Lithium. *Physical Review*, **1967**, 157, 93-96		45
7	Improved Quantum Theory of Many-Electron Systems. I. Construction of Eigenfunctions ofS^2Which Satisfy Pauli's Principle. *Physical Review*, **1967**, 157, 73-80		206
6	Improved Quantum Theory of Many-Electron Systems. II. The Basic Method. *Physical Review*, **1967**, 157, 81-93		236
5	Immobilization of □apping Arene□Cobalt(II) Complexes on Ordered Mesoporous Carbon for Electrocatalytic Water Oxidation. *ACS Catalysis*,15068-15082	13.1	2
4	Normal and Multibody Modes: Computational Analysis3399-3407		
3	Transport properties of imidazolium based ionic liquid electrolytes from molecular dynamics simulations. *Electrochemical Science Advances*,e2100007		1
2	Manganese Catalyzed Partial Oxidation of Light Alkanes. *ACS Catalysis*,5356-5370	13.1	4
1	Selective Enhancement of Methane Formation in Electrochemical CO2 Reduction Enabled by a Raman-Inactive Oxygen-Containing Species on Cu. *ACS Catalysis*,6036-6046	13.1	2