De-en Jiang

List of Publications by Year in Descending Order

361 papers	20,390 citations	79 h-index	127 g-index
386 ext. papers	23,611 ext. citations	8.8 avg, IF	7.5 L-index

#	Paper	IF	Citations
361	Sodium storage in triazine-based molecular organic electrodes: The importance of hydroxyl substituents. *Chemical Engineering Journal*, **2022**, 430, 133055	14.7	4
360	TaTiOx nanoparticles as radical scavengers to improve the durability of FeNC oxygen reduction catalysts. *Nature Energy*, **2022**, 7, 281-289	62.3	13
359	A Heteroleptic Gold Hydride Nanocluster for Efficient and Selective Electrocatalytic Reduction of CO to CO.. *Journal of the American Chemical Society*, **2022**,	16.4	9
358	Structural transformation and catalytic hydrogenation activity of amidinate-protected copper hydride clusters.. *Nature Communications*, **2022**, 13, 2082	17.4	3
357	Measuring and directing charge transfer in heterogenous catalysts. *Nature Communications*, **2022**, 13,	17.4	2
356	Band Gap as a Novel Descriptor for the Reactivity of 2D Titanium Dioxide and its Supported Pt Single Atom for Methane Activation. *Journal of Physical Chemistry Letters*, **2021**, 12, 2484-2488	6.4	4
355	Electrocatalytic synthesis of heterocycles from biomass-derived furfuryl alcohols. *Nature Communications*, **2021**, 12, 1868	17.4	7
354	Deep Learning Accelerated Determination of Hydride Locations in Metal Nanoclusters. *Angewandte Chemie - International Edition*, **2021**, 60, 12289-12292	16.4	8
353	Deep Learning Accelerated Determination of Hydride Locations in Metal Nanoclusters. *Angewandte Chemie*, **2021**, 133, 12397-12400	3.6	
352	Benzene Ring Knitting Achieved by Ambient-Temperature Dehalogenation via Mechanochemical Ullmann-Type Reductive Coupling. *Advanced Materials*, **2021**, 33, e2008685	24	12
351	Facile Cr3+-Doping Strategy Dramatically Promoting Ru/CeO2 for Low-Temperature CO2 Methanation: Unraveling the Roles of Surface Oxygen Vacancies and Hydroxyl Groups. *ACS Catalysis*, **2021**, 11, 5762-5775	13.1	17
350	Design of Graphene/Ionic Liquid Composites for Carbon Capture. *ACS Applied Materials & Interfaces*, **2021**, 13, 17511-17516	9.5	5
349	Fabrication of Ionic Covalent Triazine Framework-Linked Membranes via a Facile SolGel Approach. *Chemistry of Materials*, **2021**, 33, 3386-3393	9.6	7
348	Synthesis and Characterization of Macrocyclic Ionic Liquids for CO2 Separation. *Industrial & Engineering Chemistry Research*, **2021**, 60, 8218-8226	3.9	1
347	Revealing the etching process of water-soluble Au nanoclusters at the molecular level. *Nature Communications*, **2021**, 12, 3212	17.4	8
346	Optimal Linear Water Density for Proton Transport in Tunnel Oxides. *Journal of Physical Chemistry C*, **2021**, 125, 11508-11512	3.8	0
345	Interfacial charge transfer and interaction in the MXene/TiO2 heterostructures. *Physical Review Materials*, **2021**, 5,	3.2	4

344	CO Chemisorption Behavior of Coordination-Derived Phenolate Sorbents. *ChemSusChem*, **2021**, 14, 2854-2859	8.3	2
343	Molecular Dynamics Simulations of Complexation of Am(III) with a Preorganized Dicationic Ligand in an Ionic Liquid. *Journal of Physical Chemistry B*, **2021**, 125, 8532-8538	3.4	1
342	In Situ Strong Metal–Support Interaction (SMSI) Affects Catalytic Alcohol Conversion. *ACS Catalysis*, **2021**, 11, 1938-1945	13.1	13
341	Understanding Superatomic Ag Nanohydrides. *Small*, **2021**, 17, e2004808	11	2
340	Understanding the interaction between carboxylates and coinage metals from first principles. *Journal of Chemical Physics*, **2021**, 155, 034301	3.9	0
339	CO Chemisorption Behavior of Coordination-Derived Phenolate Sorbents. *ChemSusChem*, **2021**, 14, 2784	8.3	0
338	Fundamental Flaw in the Current Construction of the TiO Electron Transport Layer of Perovskite Solar Cells and Its Elimination. *ACS Applied Materials & Interfaces*, **2021**, 13, 39371-39378	9.5	1
337	Titanium Carbide MXene Shows an Electrochemical Anomaly in Water-in-Salt Electrolytes. *ACS Nano*, **2021**, 15, 15274-15284	16.7	18
336	Molecular dynamics simulations of a dicationic ionic liquid for CO2 capture. *Journal of Molecular Liquids*, **2021**, 335, 116163	6	1
335	Effects of interlayer confinement and hydration on capacitive charge storage in birnessite. *Nature Materials*, **2021**, 20, 1689-1694	27	21
334	Locating Hydrides in Ligand-Protected Copper Nanoclusters by Deep Learning. *ACS Applied Materials & Interfaces*, **2021**, 13, 53468-53474	9.5	1
333	Single-Atom High-Temperature Catalysis on a RhO Cluster for Production of Syngas from Methane. *Journal of the American Chemical Society*, **2021**, 143, 16566-16579	16.4	4
332	Benchmark CO2 separation achieved by highly fluorinated nanoporous molecular sieve membranes from nonporous precursor via in situ cross-linking. *Journal of Membrane Science*, **2021**, 638, 119698	9.6	1
331	Proton dynamics in water confined at the interface of the graphene-MXene heterostructure.. *Journal of Chemical Physics*, **2021**, 155, 234707	3.9	0
330	First-principles study of heterostructures of MXene and nitrogen-doped graphene as anode materials for Li-ion batteries. *Surfaces and Interfaces*, **2020**, 21, 100788	4.1	2
329	Prediction by Convolutional Neural Networks of CO2/N2 Selectivity in Porous Carbons from N2 Adsorption Isotherm at 77 K. *Angewandte Chemie*, **2020**, 132, 19813-19816	3.6	4
328	Harnessing strong metal-support interactions via a reverse route. *Nature Communications*, **2020**, 11, 3042	17.4	33
327	Prediction by Convolutional Neural Networks of CO /N Selectivity in Porous Carbons from N Adsorption Isotherm at 77 K. *Angewandte Chemie - International Edition*, **2020**, 59, 19645-19648	16.4	12

326	Interactions between Ultrastable NaAg(SR) Nanoclusters and Coordinating Solvents: Uncovering the Atomic-Scale Mechanism. *ACS Nano*, **2020**, 14, 8433-8441	16.7	9
325	Nature of Terminating Hydroxyl Groups and Intercalating Water in Ti3C2Tx MXenes: A Study by 1H Solid-State NMR and DFT Calculations. *Journal of Physical Chemistry C*, **2020**, 124, 13649-13655	3.8	19
324	Highly efficient electrocatalytic hydrogen evolution promoted by O-Mo-C interfaces of ultrafine β-Mo2C nanostructures. *Chemical Science*, **2020**, 11, 3523-3530	9.4	29
323	Transformation Strategy for Highly Crystalline Covalent Triazine Frameworks: From Staggered AB to Eclipsed AA Stacking. *Journal of the American Chemical Society*, **2020**, 142, 6856-6860	16.4	53
322	Ion-gated carbon molecular sieve gas separation membranes. *Journal of Membrane Science*, **2020**, 604, 118013	9.6	9
321	Pseudocapacitance: From Fundamental Understanding to High Power Energy Storage Materials. *Chemical Reviews*, **2020**, 120, 6738-6782	68.1	402
320	Mechanochemical synthesis of pillar[5]quinone derived multi-microporous organic polymers for radioactive organic iodide capture and storage. *Nature Communications*, **2020**, 11, 1086	17.4	38
319	The interplay between surface facet and reconstruction on isopropanol conversion over SrTiO3 nanocrystals. *Journal of Catalysis*, **2020**, 384, 49-60	7.3	7
318	Perovskite-supported Pt single atoms for methane activation. *Journal of Materials Chemistry A*, **2020**, 8, 4362-4368	13	14
317	Surpassing Robeson Upper Limit for CO2/N2 Separation with Fluorinated Carbon Molecular Sieve Membranes. *CheM*, **2020**, 6, 631-645	16.2	22
316	Interlayer separation in hydrogen titanates enables electrochemical proton intercalation. *Journal of Materials Chemistry A*, **2020**, 8, 412-421	13	19
315	Understanding hydrogen in perovskites from first principles. *Computational Materials Science*, **2020**, 174, 109461	3.2	8
314	Molecular dynamics simulations of structural and transport properties of molten NaCl-UCl3 using the polarizable-ion model. *Journal of Molecular Liquids*, **2020**, 299, 112184	6	22
313	Poly(Amidoamine) Dendrimers for Carbon Capture **2020**, 267-296		
312	Ionic Liquid-Based Membranes **2020**, 317-345		1
311	CO2 Capture and Separation of Metal–Organic Frameworks **2020**, 5-27		8
310	Porous Carbon Materials **2020**, 29-95		2
309	Porous Aromatic Frameworks for Carbon Dioxide Capture **2020**, 97-115		1

308	Virtual Screening of Materials for Carbon Capture **2020**, 117-151		2
307	Ultrathin Membranes for Gas Separation **2020**, 153-185		0
306	Polymeric Membranes **2020**, 187-214		
305	Carbon Membranes for CO2 Separation **2020**, 215-236		
304	Composite Materials for Carbon Capture **2020**, 237-266		3
303	Proton Redox and Transport in MXene-Confined Water. *ACS Applied Materials & Interfaces*, **2020**, 12, 763-770	9.5	18
302	Ionic Liquids for Chemisorption of CO2 **2020**, 297-315		2
301	Transforming Porous Organic Cages into Porous Ionic Liquids via a Supramolecular Complexation Strategy. *Angewandte Chemie*, **2020**, 132, 2288-2292	3.6	9
300	Transforming Porous Organic Cages into Porous Ionic Liquids via a Supramolecular Complexation Strategy. *Angewandte Chemie - International Edition*, **2020**, 59, 2268-2272	16.4	50
299	Ethanol Conversion over La0.7Sr0.3MnO3□(100): Autocatalysis, Adjacent O-Vacancies, Disproportionation, and Dehydrogenation. *ACS Catalysis*, **2020**, 10, 12920-12931	13.1	3
298	Electrode material□onic liquid coupling for electrochemical energy storage. *Nature Reviews Materials*, **2020**, 5, 787-808	73.3	89
297	Hydrogen in Nanocatalysis. *Journal of Physical Chemistry Letters*, **2020**, 11, 7049-7057	6.4	10
296	Descriptors for Hydrogen Evolution on Single Atom Catalysts in Nitrogen-Doped Graphene. *Journal of Physical Chemistry C*, **2020**, 124, 19571-19578	3.8	20
295	Control of single-ligand chemistry on thiolated Au nanoclusters. *Nature Communications*, **2020**, 11, 5498	17.4	23
294	All-Carboxylate-Protected Superatomic Silver Nanocluster with an Unprecedented Rhombohedral Ag Core. *Journal of the American Chemical Society*, **2020**, 142, 16905-16909	16.4	40
293	Stable Surface Terminations of a Perovskite Oxyhydride from First-Principles. *Journal of Physical Chemistry C*, **2020**, 124, 18557-18563	3.8	0
292	Sinter-Resistant Nanoparticle Catalysts Achieved by 2D Boron Nitride-Based Strong Metal-Support Interactions: A New Twist on an Old Story. *ACS Central Science*, **2020**, 6, 1617-1627	16.8	15
291	Structure and Dynamics of Aqueous Electrolytes Confined in 2D-TiO/TiCT MXene Heterostructures. *ACS Applied Materials & Interfaces*, **2020**, 12, 58378-58389	9.5	4

290	Understanding the conversion of ethanol to propene on In2O3 from first principles. *Catalysis Today*, **2020**, 350, 19-24	5.3	6
289	A new trick for an old support: Stabilizing gold single atoms on LaFeO3 perovskite. *Applied Catalysis B: Environmental*, **2020**, 261, 118178	21.8	21
288	Porous liquid zeolites: hydrogen bonding-stabilized H-ZSM-5 in branched ionic liquids. *Nanoscale*, **2019**, 11, 1515-1519	7.7	52
287	Computational screening of M/Cu core/shell nanoparticles and their applications for the electro-chemical reduction of CO and CO. *Nanoscale*, **2019**, 11, 11351-11359	7.7	5
286	Effect of Hydrogen-Induced Metallization on Chemisorption. *Journal of Physical Chemistry C*, **2019**, 123, 15171-15175	3.8	2
285	Computational Discovery and Design of MXenes for Energy Applications: Status, Successes, and Opportunities. *ACS Applied Materials & Interfaces*, **2019**, 11, 24885-24905	9.5	65
284	Phosphorene-Supported Transition-Metal Dimer for Effective N Electroreduction. *ChemPhysChem*, **2019**, 20, 3141-3146	3.2	14
283	Elucidation of the Reaction Mechanism for High-Temperature Water Gas Shift over an Industrial-Type Copper-Chromium-Iron Oxide Catalyst. *Journal of the American Chemical Society*, **2019**, 141, 7990-7999	16.4	33
282	Efficient Absorption of SO2 by Deep Eutectic Solvents Formed by Biobased Aprotic Organic Compound Succinonitrile and 1-Ethyl-3-methylimidazolium Chloride. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 9086-9091	8.3	42
281	Highly Polar but Amorphous Polymers with Robust Membrane CO2/N2 Separation Performance. *Joule*, **2019**, 3, 1881-1894	27.8	30
280	Topotactic Synthesis of Phosphabenzene-Functionalized Porous Organic Polymers: Efficient Ligands in CO2 Conversion. *Angewandte Chemie*, **2019**, 131, 13901-13905	3.6	2
279	Methane Chemisorption on Oxide-Supported Pt Single Atom. *ChemPhysChem*, **2019**, 20, 2217-2220	3.2	9
278	Topotactic Synthesis of Phosphabenzene-Functionalized Porous Organic Polymers: Efficient Ligands in CO Conversion. *Angewandte Chemie - International Edition*, **2019**, 58, 13763-13767	16.4	18
277	Entropic selectivity in air separation via a bilayer nanoporous graphene membrane. *Physical Chemistry Chemical Physics*, **2019**, 21, 16310-16315	3.6	3
276	Influence of fluorination on CO2 adsorption in materials derived from fluorinated covalent triazine framework precursors. *Journal of Materials Chemistry A*, **2019**, 7, 17277-17282	13	30
275	Insights into CO2/N2 Selectivity in Porous Carbons from Deep Learning **2019**, 1, 558-563		16
274	Real Time Monitoring of the Dynamic Intracluster Diffusion of Single Gold Atoms into Silver Nanoclusters. *Journal of the American Chemical Society*, **2019**, 141, 18977-18983	16.4	48
273	Confined Interlayer Water Promotes Structural Stability for High-Rate Electrochemical Proton Intercalation in Tungsten Oxide Hydrates. *ACS Energy Letters*, **2019**, 4, 2805-2812	20.1	51

272	Three-orders-of-magnitude variation of carrier lifetimes with crystal phase of gold nanoclusters. *Science*, **2019**, 364, 279-282	33.3	75
271	Interfacial and electronic properties of heterostructures of MXene and graphene. *Physical Review B* , **2019**, 99,	3.3	34
270	First-Principles Molecular Dynamics Simulations of UCln NaCl (n = 3, 4) Molten Salts. *ACS Applied Energy Materials*, **2019**, 2, 2122-2128	6.1	24
269	Density-Functional Tight-Binding for Platinum Clusters and Bulk: Electronic vs Repulsive Parameters. *MRS Advances*, **2019**, 4, 1821-1832	0.7	1
268	Continuously Tunable Pore Size for Gas Separation via a Bilayer Nanoporous Graphene Membrane. *ACS Applied Nano Materials*, **2019**, 2, 379-384	5.6	22
267	Deep eutectic solvents formed by quaternary ammonium salts and aprotic organic compound succinonitrile. *Journal of Molecular Liquids*, **2019**, 274, 414-417	6	10
266	Confined Ionic Liquid in an Ionic Porous Aromatic Framework for Gas Separation. *ACS Applied Polymer Materials*, **2019**, 1, 95-102	4.3	13
265	Structure and Interaction of Ionic Liquid Monolayer on Graphite from First-Principles. *Journal of Physical Chemistry C*, **2019**, 123, 618-624	3.8	8
264	Computational Screening of MXene Electrodes for Pseudocapacitive Energy Storage. *Journal of Physical Chemistry C*, **2019**, 123, 315-321	3.8	47
263	Understanding the MXene Pseudocapacitance. *Journal of Physical Chemistry Letters*, **2018**, 9, 1223-1228	6.4	133
262	Fluorescence of Hydroxyphenyl-Substituted "Click" Triazoles. *Journal of Physical Chemistry A*, **2018**, 122, 2956-2973	2.8	18
261	Selective CO Production by Photoelectrochemical Methane Oxidation on TiO. *ACS Central Science*, **2018**, 4, 631-637	16.8	30
260	Carbon Dioxide Separation: Highly Permeable Oligo(ethylene oxide)-co-poly(dimethylsiloxane) Membranes for Carbon Dioxide Separation (Adv. Sustainable Syst. 4/2018). *Advanced Sustainable Systems*, **2018**, 2, 1870030	5.9	1
259	Universal molecular-confined synthesis of interconnected porous metal oxides-N-C frameworks for electrocatalytic water splitting. *Nano Energy*, **2018**, 48, 600-606	17.1	50
258	Displacement of carbonates in CaUO(CO) by amidoxime-based ligands from free-energy simulations. *Dalton Transactions*, **2018**, 47, 1604-1613	4.3	1
257	Interface Engineering of Earth-Abundant Transition Metals Using Boron Nitride for Selective Electroreduction of CO. *ACS Applied Materials & Interfaces*, **2018**, 10, 6694-6700	9.5	40
256	Dopant-Dependent Electronic Structures Observed for MAu(SCH) Clusters (M = Pt, Pd). *Journal of Physical Chemistry Letters*, **2018**, 9, 982-989	6.4	37
255	Highly Permeable Oligo(ethylene oxide)-co-poly(dimethylsiloxane) Membranes for Carbon Dioxide Separation. *Advanced Sustainable Systems*, **2018**, 2, 1700113	5.9	4

254	Thiolate-Protected Trimetallic AuAgPd and AuAgPt Alloy Clusters with Controlled Chemical Composition and Metal Positions. *Journal of Physical Chemistry Letters*, **2018**, 9, 2590-2594	6.4	38
253	SO absorption in EmimCl-TEG deep eutectic solvents. *Physical Chemistry Chemical Physics*, **2018**, 20, 15168-15173	3.8	33
252	Single rhodium atoms anchored in micropores for efficient transformation of methane under mild conditions. *Nature Communications*, **2018**, 9, 1231	17.4	140
251	Understanding Methanol Coupling on SrTiO3 from First Principles. *Journal of Physical Chemistry C*, **2018**, 122, 7210-7216	3.8	1
250	Stronger-than-Pt hydrogen adsorption in a Au22 nanocluster for the hydrogen evolution reaction. *Journal of Materials Chemistry A*, **2018**, 6, 7532-7537	13	41
249	Trends of Alkane Activation on Doped Cobalt (II, III) Oxide from First Principles. *ChemCatChem*, **2018**, 10, 244-249	5.2	17
248	Effect of pore density on gas permeation through nanoporous graphene membranes. *Nanoscale*, **2018**, 10, 14660-14666	7.7	23
247	First-Principles Insight into Electrocatalytic Reduction of CO2 to CH4 on a Copper Nanoparticle. *Journal of Physical Chemistry C*, **2018**, 122, 11392-11398	3.8	39
246	Low-temperature activation of methane on doped single atoms: descriptor and prediction. *Physical Chemistry Chemical Physics*, **2018**, 20, 22909-22914	3.6	40
245	Supported bicyclic amidine ionic liquids as a potential CO2/N2 separation medium. *Journal of Membrane Science*, **2018**, 565, 203-212	9.6	20
244	First Principles Insight into H2 Activation and Hydride Species on TiO2 Surfaces. *Journal of Physical Chemistry C*, **2018**, 122, 20323-20328	3.8	21
243	Hetero-biicosahedral [AuPd(PPh)(SCHPh)Cl] nanocluster: selective synthesis and optical and electrochemical properties. *Nanoscale*, **2018**, 10, 18969-18979	7.7	35
242	Synthesis of Water-Soluble [Au(SR)] Using a Stoichiometric Amount of NaBH. *Journal of the American Chemical Society*, **2018**, 140, 11370-11377	16.4	72
241	Exploring perovskites for methane activation from first principles. *Catalysis Science and Technology*, **2018**, 8, 702-709	5.5	22
240	Insights into Interfaces, Stability, Electronic Properties, and Catalytic Activities of Atomically Precise Metal Nanoclusters from First Principles. *Accounts of Chemical Research*, **2018**, 51, 2793-2802	24.3	156
239	Understanding the Binding of a Bifunctional Amidoximate-Carboxylate Ligand with Uranyl in Seawater. *Journal of Physical Chemistry B*, **2018**, 122, 12060-12066	3.4	2
238	Effects of Metal-Doping on Hydrogen Evolution Reaction Catalyzed by MAu and MAu Nanoclusters (M = Pt, Pd). *ACS Applied Materials & Interfaces*, **2018**, 10, 44645-44653	9.5	57
237	Rationally designed metal nanocluster for electrocatalytic hydrogen production from water. *Journal of Materials Chemistry A*, **2018**, 6, 19495-19501	13	25

236	Understanding the Impact of Surface Reconstruction of Perovskite Catalysts on CH4 Activation and Combustion. *ACS Catalysis*, **2018**, 8, 10306-10315	13.1	36
235	Golden single-atomic-site platinum electrocatalysts. *Nature Materials*, **2018**, 17, 1033-1039	27	177
234	Origins and Implications of Interfacial Capacitance Enhancements in C-Modified Graphene Supercapacitors. *ACS Applied Materials & Interfaces*, **2018**, 10, 36860-36865	9.5	19
233	New Bonding Model of Radical Adsorbate on Lattice Oxygen of Perovskites. *Journal of Physical Chemistry Letters*, **2018**, 9, 6321-6325	6.4	21
232	Revealing isoelectronic size conversion dynamics of metal nanoclusters by a noncrystallization approach. *Nature Communications*, **2018**, 9, 1979	17.4	75
231	Promotion of catalytic selectivity on transition metal oxide through restructuring surface lattice. *Applied Catalysis B: Environmental*, **2018**, 237, 957-969	21.8	15
230	Exploring Structural Diversity and Fluxionality of Ptn (n = 10□13) Clusters from First-Principles. *Journal of Physical Chemistry C*, **2017**, 121, 10796-10802	3.8	21
229	Computational insight into the capacitive performance of graphene edge planes. *Carbon*, **2017**, 116, 278-285	10.4	28
228	Hydrogen functionalisation of transition metal dichalcogenide monolayers from first principles. *Molecular Simulation*, **2017**, 43, 379-383	2	6
227	Impact of tuning CO2-philicity in polydimethylsiloxane-based membranes for carbon dioxide separation. *Journal of Membrane Science*, **2017**, 530, 213-219	9.6	21
226	Ion-Gated Gas Separation through Porous Graphene. *Nano Letters*, **2017**, 17, 1802-1807	11.5	84
225	A molecule-like PtAu(SCH) nanocluster as an electrocatalyst for hydrogen production. *Nature Communications*, **2017**, 8, 14723	17.4	196
224	Computational Insights into Materials and Interfaces for Capacitive Energy Storage. *Advanced Science*, **2017**, 4, 1700059	13.6	122
223	Metallic Hydrogen in Atomically Precise Gold Nanoclusters. *Chemistry of Materials*, **2017**, 29, 4840-4847	9.6	54
222	General Structure-Reactivity Relationship for Oxygen on Transition-Metal Oxides. *Journal of Physical Chemistry Letters*, **2017**, 8, 2206-2211	6.4	49
221	Highly Efficient Carbon Monoxide Capture by Carbanion-Functionalized Ionic Liquids through C-Site Interactions. *Angewandte Chemie*, **2017**, 129, 6947-6951	3.6	22
220	R□cktitelbild: Highly Efficient Carbon Monoxide Capture by Carbanion-Functionalized Ionic Liquids through C-Site Interactions (Angew. Chem. 24/2017). *Angewandte Chemie*, **2017**, 129, 7108-7108	3.6	
219	Highly Efficient Carbon Monoxide Capture by Carbanion-Functionalized Ionic Liquids through C-Site Interactions. *Angewandte Chemie - International Edition*, **2017**, 56, 6843-6847	16.4	63

218	Pd-Metalated Conjugated Nanoporous Polycarbazoles for Additive-Free Cyanation of Aryl Halides: Boosting Catalytic Efficiency through Spatial Modulation. *ChemSusChem*, **2017**, 10, 2320-2320	8.3	
217	Controlling Reaction Selectivity through the Surface Termination of Perovskite Catalysts. *Angewandte Chemie*, **2017**, 129, 9952-9956	3.6	16
216	Controlling Reaction Selectivity through the Surface Termination of Perovskite Catalysts. *Angewandte Chemie - International Edition*, **2017**, 56, 9820-9824	16.4	30
215	Lattice-Hydride Mechanism in Electrocatalytic CO Reduction by Structurally Precise Copper-Hydride Nanoclusters. *Journal of the American Chemical Society*, **2017**, 139, 9728-9736	16.4	164
214	Alkynyl-protected silver nanoclusters featuring an anticuboctahedral kernel. *Nanoscale*, **2017**, 9, 11405-11409	7.4	54
213	Acid–Base Reactivity of Perovskite Catalysts Probed via Conversion of 2-Propanol over Titanates and Zirconates. *ACS Catalysis*, **2017**, 7, 4423-4434	13.1	49
212	Capacitive Energy Extraction by Few-Layer Graphene Electrodes. *Journal of Physical Chemistry C*, **2017**, 121, 14010-14018	3.8	18
211	Pd-Metalated Conjugated Nanoporous Polycarbazoles for Additive-Free Cyanation of Aryl Halides: Boosting Catalytic Efficiency through Spatial Modulation. *ChemSusChem*, **2017**, 10, 2348-2351	8.3	12
210	Design of Calix-Based Cages for CO2 Capture. *Industrial & Engineering Chemistry Research*, **2017**, 56, 4502-4507	3.9	6
209	Solvation of the vanadate ion in seawater conditions from molecular dynamics simulations. *Inorganica Chimica Acta*, **2017**, 458, 39-44	2.7	6
208	Solvent Polarity Governs Ion Interactions and Transport in a Solvated Room-Temperature Ionic Liquid. *Journal of Physical Chemistry Letters*, **2017**, 8, 167-171	6.4	35
207	Understanding seed-mediated growth of gold nanoclusters at molecular level. *Nature Communications*, **2017**, 8, 927	17.4	178
206	Optimal Size of a Cylindrical Pore for Post-Combustion CO2 Capture. *Journal of Physical Chemistry C* , **2017**, 121, 22025-22030	3.8	7
205	Identify the Removable Substructure in Carbon Activation. *Chemistry of Materials*, **2017**, 29, 7288-7295	9.6	38
204	Comprehensive View of the Ligand–Gold Interface from First Principles. *Chemistry of Materials*, **2017**, 29, 6908-6915	9.6	46
203	Effect of Salt on the Uranyl Binding with Carbonate and Calcium Ions in Aqueous Solutions. *Journal of Physical Chemistry B*, **2017**, 121, 8171-8178	3.4	11
202	Uranyl-Glutardiamidoxime Binding from First-Principles Molecular Dynamics, Classical Molecular Dynamics, and Free-Energy Simulations. *Inorganic Chemistry*, **2017**, 56, 9497-9504	5.1	6
201	Universal Surface Engineering of Transition Metals for Superior Electrocatalytic Hydrogen Evolution in Neutral Water. *Journal of the American Chemical Society*, **2017**, 139, 12283-12290	16.4	151

200	Selective Charging Behavior in an Ionic Mixture Electrolyte-Supercapacitor System for Higher Energy and Power. *Journal of the American Chemical Society*, **2017**, 139, 18681-18687	16.4	76
199	Precise control of alloying sites of bimetallic nanoclusters via surface motif exchange reaction. *Nature Communications*, **2017**, 8, 1555	17.4	100
198	Kinetics and Mechanism of Methanol Conversion over Anatase Titania Nanoshapes. *ACS Catalysis*, **2017**, 7, 5345-5356	13.1	24
197	Atomically Precise Bimetallic AuCu Nanocluster with an Icosidodecahedral Cu Shell and an Alkynyl-Cu Interface. *Journal of the American Chemical Society*, **2017**, 139, 9451-9454	16.4	79
196	Computational Insight into the Covalent Organic□norganic Interface. *Chemistry of Materials*, **2016**, 28, 5976-5988	9.6	22
195	CoP for hydrogen evolution: implications from hydrogen adsorption. *Physical Chemistry Chemical Physics*, **2016**, 18, 23864-71	3.6	64
194	Substitution Effect Guided Synthesis of Task-Specific Nanoporous Polycarbazoles with Enhanced Carbon Capture. *Macromolecules*, **2016**, 49, 5325-5330	5.5	32
193	Solvation of the Ca2UO2(CO3)3 Complex in Seawater from Classical Molecular Dynamics. *Journal of Physical Chemistry B*, **2016**, 120, 7227-33	3.4	12
192	Boron Supercapacitors. *ACS Energy Letters*, **2016**, 1, 1241-1246	20.1	52
191	Understanding the pseudocapacitance of RuO2 from joint density functional theory. *Journal of Physics Condensed Matter*, **2016**, 28, 464004	1.8	20
190	What can molecular simulation do for global warming?. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2016**, 6, 173-197	7.9	28
189	Tuning Catalytic Selectivity of Oxidative Catalysis through Deposition of Nonmetallic Atoms in Surface Lattice of Metal Oxide. *ACS Catalysis*, **2016**, 6, 4218-4228	13.1	28
188	Mechanism of Hydrogen Evolution Reaction on 1T-MoS2 from First Principles. *ACS Catalysis*, **2016**, 6, 4953-4961	13.1	489
187	Site Partition: Turning One Site into Two for Adsorbing CO2. *Journal of Physical Chemistry Letters*, **2016**, 7, 2568-72	6.4	15
186	Multi-Molar Absorption of CO2 by the Activation of Carboxylate Groups in Amino Acid Ionic Liquids. *Angewandte Chemie*, **2016**, 128, 7282-7286	3.6	35
185	Enhancing graphene capacitance by nitrogen: effects of doping configuration and concentration. *Physical Chemistry Chemical Physics*, **2016**, 18, 4668-74	3.6	84
184	Isomerism in Au28(SR)20 Nanocluster and Stable Structures. *Journal of the American Chemical Society*, **2016**, 138, 1482-5	16.4	202
183	Contribution of Dielectric Screening to the Total Capacitance of Few-Layer Graphene Electrodes. *Journal of Physical Chemistry Letters*, **2016**, 7, 789-94	6.4	33

182	Rational design and synthesis of a porous, task-specific polycarbazole for efficient CO2 capture. *Chemical Communications*, **2016**, 52, 4454-7	5.8	47
181	First-principles molecular dynamics simulation of the Ca2UO2(CO3)3 complex in water. *Dalton Transactions*, **2016**, 45, 9812-9	4.3	20
180	A Poly(acrylonitrile)-Functionalized Porous Aromatic Framework Synthesized by Atom-Transfer Radical Polymerization for the Extraction of Uranium from Seawater. *Industrial & Engineering Chemistry Research*, **2016**, 55, 4125-4129	3.9	42
179	Nickel sulfides for electrocatalytic hydrogen evolution under alkaline conditions: a case study of crystalline NiS, NiS2, and Ni3S2 nanoparticles. *Catalysis Science and Technology*, **2016**, 6, 1077-1084	5.5	330
178	Multi-Molar Absorption of CO2 by the Activation of Carboxylate Groups in Amino Acid Ionic Liquids. *Angewandte Chemie - International Edition*, **2016**, 55, 7166-70	16.4	212
177	Efficient adsorptive desulfurization by task-specific porous organic polymers. *AICHE Journal*, **2016**, 62, 1740-1746	3.6	23
176	Beyond the staple motif: a new order at the thiolate-gold interface. *Nanoscale*, **2016**, 8, 20103-20110	7.7	27
175	The N-B Interaction through a Water Bridge: Understanding the Chemoselectivity of a Fluorescent Protein Based Probe for Peroxynitrite. *Journal of the American Chemical Society*, **2016**, 138, 4900-7	16.4	49
174	Understanding oxidative dehydrogenation of ethane on Co3O4 nanorods from density functional theory. *Catalysis Science and Technology*, **2016**, 6, 6861-6869	5.5	30
173	Comparative Reaction Diagrams for the SN(2) Reaction Formulated According to the Leffler Analysis and the Hammond Postulate. *Journal of Organic Chemistry*, **2016**, 81, 3648-53	4.2	4
172	A Generic Model for Electric Double Layers in Porous Electrodes. *Journal of Physical Chemistry C*, **2016**, 120, 8704-8710	3.8	57
171	Enhancing the Capacitive Performance of Electric Double-Layer Capacitors with Ionic Liquid Mixtures. *ACS Energy Letters*, **2016**, 1, 21-26	20.1	107
170	Use of steric encumbrance to develop conjugated nanoporous polymers for metal-free catalytic hydrogenation. *Chemical Communications*, **2016**, 52, 11919-11922	5.8	11
169	Diphosphine-Protected Au Nanoclusters on Oxide Supports Are Active for Gas-Phase Catalysis without Ligand Removal. *Nano Letters*, **2016**, 16, 6560-6567	11.5	70
168	Interconversion between Superatomic 6-Electron and 8-Electron Configurations of M@Au[SR] Clusters (M = Pd, Pt). *Journal of the American Chemical Society*, **2015**, 137, 10833-40	16.4	146
167	Stability and Core-Level Signature of Nitrogen Dopants in Carbonaceous Materials. *Chemistry of Materials*, **2015**, 27, 5775-5781	9.6	29
166	Ag29(BDT)12(TPP)4: A Tetravalent Nanocluster. *Journal of the American Chemical Society*, **2015**, 137, 11970-5	16.4	284
165	The surface structure of silver-coated gold nanocrystals and its influence on shape control. *Nature Communications*, **2015**, 6, 7664	17.4	50

164	Structural Evolution of Tcn (n = 4-20) Clusters from First-Principles Global Minimization. *Journal of Physical Chemistry A*, **2015**, 119, 8892-7	2.8	9
163	Expanded Porphyrins as Two-Dimensional Porous Membranes for CO2 Separation. *ACS Applied Materials & Interfaces*, **2015**, 7, 13073-9	9.5	55
162	Stabilization and Band-Gap Tuning of the 1T-MoS2 Monolayer by Covalent Functionalization. *Chemistry of Materials*, **2015**, 27, 3743-3748	9.6	211
161	Ab Initio Screening of CO2-philic Groups. *Journal of Physical Chemistry A*, **2015**, 119, 3848-52	2.8	24
160	Alkynyl-protected Au23 nanocluster: a 12-electron system. *Angewandte Chemie - International Edition*, **2015**, 54, 5977-80	16.4	114
159	Theoretic Insights into Porous Carbon-Based Supercapacitors **2015**, 361-378		1
158	Understanding Selective Hydrogenation of □Unsaturated Ketones to Unsaturated Alcohols on the Au25(SR)18 Cluster. *ACS Catalysis*, **2015**, 5, 6624-6629	13.1	56
157	Global minimization of gold clusters by combining neural network potentials and the basin-hopping method. *Nanoscale*, **2015**, 7, 14817-21	7.7	64
156	Theoretical investigation on two-dimensional non-traditional carbon materials employing three-membered ring and four-membered ring as building blocks. *Carbon*, **2015**, 95, 1033-1038	10.4	18
155	Quantum Effects on the Capacitance of Graphene-Based Electrodes. *Journal of Physical Chemistry C* , **2015**, 119, 22297-22303	3.8	92
154	Ligand-Conformation Energy Landscape of Thiolate-Protected Gold Nanoclusters. *Journal of Physical Chemistry C*, **2015**, 119, 21555-21560	3.8	18
153	Insights into the PhC?C/Au Interface. *Journal of Physical Chemistry C*, **2015**, 119, 10804-10810	3.8	45
152	The ligand effect on the isomer stability of Au24(SR)20 clusters. *Nanoscale*, **2015**, 7, 2225-9	7.7	50
151	Absorption and Emission Sensitivity of 2-(2'-Hydroxyphenyl)benzoxazole to Solvents and Impurities. *Photochemistry and Photobiology*, **2015**, 91, 586-98	3.6	22
150	Selectivity trend of gas separation through nanoporous graphene. *Journal of Solid State Chemistry*, **2015**, 224, 2-6	3.3	77
149	Nitrogen-doped porous aromatic frameworks for enhanced CO2 adsorption. *Journal of Colloid and Interface Science*, **2015**, 438, 191-195	9.3	30
148	Effect of Cross-Link Density on Carbon Dioxide Separation in Polydimethylsiloxane-Norbornene Membranes. *ChemSusChem*, **2015**, 8, 3524-3524	8.3	2
147	Structure Prediction by Density Functional Theory Calculations. *Frontiers of Nanoscience*, **2015**, 9, 161-187	7.7	

146	Alkynyl-Protected Au23 Nanocluster: A 12-Electron System. *Angewandte Chemie*, **2015**, 127, 6075-6078	3.6	43
145	Effect of Cross-Link Density on Carbon Dioxide Separation in Polydimethylsiloxane-Norbornene Membranes. *ChemSusChem*, **2015**, 8, 3595-604	8.3	16
144	Revisiting Structural Models for Au18(SR)14. *Journal of Physical Chemistry C*, **2015**, 150127073220004	3.8	9
143	Au19 nanocluster featuring a V-shaped alkynyl-gold motif. *Journal of the American Chemical Society*, **2015**, 137, 652-5	16.4	176
142	Computational quest for spherical C12B68 fullerenes with "magic" □electrons and quasi-planar tetra-coordinated carbon. *Journal of Molecular Modeling*, **2014**, 20, 2085	2	4
141	Structure and dynamics of CO2 and N2 in a tetracyanoborate based ionic liquid. *Physical Chemistry Chemical Physics*, **2014**, 16, 1909-13	3.6	19
140	Identification of a highly luminescent Au22(SG)18 nanocluster. *Journal of the American Chemical Society*, **2014**, 136, 1246-9	16.4	436
139	Quantum mechanical basis for kinetic diameters of small gaseous molecules. *Journal of Physical Chemistry A*, **2014**, 118, 1150-4	2.8	140
138	Gold nanowired: a linear (Au25)(n) polymer from Au25 molecular clusters. *ACS Nano*, **2014**, 8, 8505-12	16.7	122
137	Unusual effects of solvent polarity on capacitance for organic electrolytes in a nanoporous electrode. *Nanoscale*, **2014**, 6, 5545-50	7.7	58
136	Kinetic Charging Inversion in Ionic Liquid Electric Double Layers. *Journal of Physical Chemistry Letters*, **2014**, 5, 2195-200	6.4	48
135	Highly soluble alkoxide magnesium salts for rechargeable magnesium batteries. *Journal of Materials Chemistry A*, **2014**, 2, 581-584	13	55
134	Solubility of gases in a common ionic liquid from molecular dynamics based free energy calculations. *Journal of Physical Chemistry B*, **2014**, 118, 2719-25	3.4	44
133	Molecular Dynamics Simulation of Anion Effect on Solubility, Diffusivity, and Permeability of Carbon Dioxide in Ionic Liquids. *Industrial & Engineering Chemistry Research*, **2014**, 53, 10485-10490	3.9	39
132	CO2 Adsorption As a Flat-Lying, Tridentate Carbonate on CeO2(100). *Journal of Physical Chemistry C*, **2014**, 118, 9042-9050	3.8	61
131	Impact of the Selenolate Ligand on the Bonding Behavior of Au25 Nanoclusters. *Journal of Physical Chemistry C*, **2014**, 118, 21730-21737	3.8	13
130	Superatomic Orbitals under Spin-Orbit Coupling. *Journal of Physical Chemistry Letters*, **2014**, 5, 3286-9	6.4	99
129	Toward understanding the growth mechanism: tracing all stable intermediate species from reduction of Au(I)-thiolate complexes to evolution of Au□nanoclusters. *Journal of the American Chemical Society*, **2014**, 136, 10577-80	16.4	255

128	Thiolate ligands as a double-edged sword for CO oxidation on CeO2 supported Au25(SCH2CH2Ph)18 nanoclusters. *Journal of the American Chemical Society*, **2014**, 136, 6111-22	16.4	215
127	Size Dependence of Atomically Precise Gold Nanoclusters in Chemoselective Hydrogenation and Active Site Structure. *ACS Catalysis*, **2014**, 4, 2463-2469	13.1	108
126	Selective deposition of Ru nanoparticles on TiSi□hanonet and its utilization for Li□□formation and decomposition. *Journal of the American Chemical Society*, **2014**, 136, 8903-6	16.4	100
125	Time-dependent density functional theory for ion diffusion in electrochemical systems. *Journal of Physics Condensed Matter*, **2014**, 26, 284102	1.8	37
124	Anion-Functionalized Task-Specific Ionic Liquids: Molecular Origin of Change in Viscosity upon CO2 Capture. *Journal of Physical Chemistry B*, **2014**, 118, 14880-7	3.4	32
123	Synthesis and Characterization of Lithium Bis(fluoromalonato)borate for Lithium-Ion Battery Applications. *Advanced Energy Materials*, **2014**, 4, 1301368	21.8	37
122	Correction to □dentification of a Highly Luminescent Au22(SG)18 Nanocluster□*Journal of the American Chemical Society*, **2014**, 136, 17355-17355	16.4	2
121	Coordination effect-regulated CO2 capture with an alkali metal onium salts/crown ether system. *Green Chemistry*, **2014**, 16, 253-258	10	30
120	Intrinsic Magnetism in Edge-Reconstructed Zigzag Graphene Nanoribbons **2013**, 9-28		
119	Understanding Aromaticity of Graphene and Graphene Nanoribbons by the Clar Sextet Rule **2013**, 29-49		4
118	Physical Properties of Graphene Nanoribbons: Insights from First-Principles Studies **2013**, 51-77		1
117	Cutting Graphitic Materials: A Promising Way to Prepare Graphene Nanoribbons **2013**, 79-99		
116	The strategies for improving carbon dioxide chemisorption by functionalized ionic liquids. *RSC Advances*, **2013**, 3, 15518	3.7	108
115	Oxide-supported atomically precise gold nanocluster for catalyzing Sonogashira cross-coupling. *Journal of Catalysis*, **2013**, 306, 177-183	7.3	97
114	Vibrational cross-angles in condensed molecules: a structural tool. *Journal of Physical Chemistry A*, **2013**, 117, 8407-15	2.8	14
113	Properties of Nanographenes **2013**, 101-127		
112	Porous Graphene and Nanomeshes **2013**, 129-151		1
111	Surface Functionalization of Graphene **2013**, 233-253		2

110	From Graphene to Graphene Oxide and Back **2013**, 291-317		2
109	Electronic Transport in Graphitic Carbon Nanoribbons **2013**, 319-346		2
108	Linking Theory to Reactivity and Properties of Nanographenes **2013**, 393-424		1
107	Graphene Moiré Supported Metal Clusters for Model Catalytic Studies **2013**, 425-446		
106	Bicyclic imidazolium ionic liquids as potential electrolytes for rechargeable lithium ion batteries. *Journal of Power Sources*, **2013**, 237, 5-12	8.9	34
105	Effect of alkyl and aryl substitutions on 1,2,4-triazolium-based ionic liquids for carbon dioxide separation and capture. *RSC Advances*, **2013**, 3, 3981	3.7	28
104	Graphitic mesoporous carbon-supported molybdenum carbides for catalytic hydrogenation of carbon monoxide to mixed alcohols. *Microporous and Mesoporous Materials*, **2013**, 170, 141-149	5.3	20
103	Permeance of H2 through porous graphene from molecular dynamics. *Solid State Communications*, **2013**, 175-176, 101-105	1.6	52
102	The expanding universe of thiolated gold nanoclusters and beyond. *Nanoscale*, **2013**, 5, 7149-60	7.7	153
101	Microscopic Insights into the Electrochemical Behavior of Nonaqueous Electrolytes in Electric Double-Layer Capacitors. *Journal of Physical Chemistry Letters*, **2013**, 4, 1260-7	6.4	95
100	Rhodium Nanoparticles Confined in Ordered Mesoporous Carbon: Microscopic Characterization and Catalytic Application for Synthesis Gas Conversion to Ethanol. *ACS Symposium Series*, **2013**, 231-243	0.4	
99	Structure of Au15(SR)13 and its implication for the origin of the nucleus in thiolated gold nanoclusters. *Journal of the American Chemical Society*, **2013**, 135, 8786-9	16.4	114
98	Insights into CO2/N2 separation through nanoporous graphene from molecular dynamics. *Nanoscale*, **2013**, 5, 9984-7	7.7	120
97	Ring-opened heterocycles: Promising ionic liquids for gas separation and capture. *Journal of Membrane Science*, **2012**, 401-402, 61-67	9.6	32
96	Solid–Electrolyte Interphase Formation and Electrolyte Reduction at Li-Ion Battery Graphite Anodes: Insights from First-Principles Molecular Dynamics. *Journal of Physical Chemistry C*, **2012**, 116, 24476-24481	3.8	94
95	Windowed Carbon Nanotubes for Efficient CO2 Removal from Natural Gas. *Journal of Physical Chemistry Letters*, **2012**, 3, 3343-3347	6.4	57
94	Solvent Effect on the Pore-Size Dependence of an Organic Electrolyte Supercapacitor. *Journal of Physical Chemistry Letters*, **2012**, 3, 1727-31	6.4	151
93	Nitrogen-Doped Mesoporous Carbon for Carbon Capture: A Molecular Simulation Study. *Journal of Physical Chemistry C*, **2012**, 116, 7106-7110	3.8	38

92	Application of density functional theory to study the double layer of an electrolyte with an explicit dimer model for the solvent. *Journal of Physical Chemistry B*, **2012**, 116, 11356-61	3.4	30
91	Monoplatinum doping of gold nanoclusters and catalytic application. *Journal of the American Chemical Society*, **2012**, 134, 16159-62	16.4	383
90	Oxidation potentials of functionalized sulfone solvents for high-voltage Li-ion batteries: a computational study. *Journal of Physical Chemistry B*, **2012**, 116, 3235-8	3.4	60
89	Structures and Energetics of Pt Clusters on TiO2: Interplay between Metal□Metal Bonds and Metal□Oxygen Bonds. *Journal of Physical Chemistry C*, **2012**, 116, 21880-21885	3.8	33
88	Mn monolayer modified Rh for syngas-to-ethanol conversion: a first-principles study. *Nanoscale*, **2012**, 4, 1123-9	7.7	29
87	High CO2 solubility, permeability and selectivity in ionic liquids with the tetracyanoborate anion. *RSC Advances*, **2012**, 2, 11813	3.7	96
86	Computer-Aided Design of Interpenetrated Tetrahydrofuran-Functionalized 3D Covalent Organic Frameworks for CO2 Capture. *Crystal Growth and Design*, **2012**, 12, 5349-5356	3.5	32
85	The halogen analogs of thiolated gold nanoclusters. *Nanoscale*, **2012**, 4, 4234-9	7.7	29
84	Aryl□Surface Bonding: A Density Functional Theory (DFT) Simulation Approach **2012**, 37-52		2
83	Curvature Effect on the Capacitance of Electric Double Layers at Ionic Liquid/Onion-Like Carbon Interfaces. *Journal of Chemical Theory and Computation*, **2012**, 8, 1058-63	6.4	104
82	Synthesis and Characterization of Thiazolium-Based Room Temperature Ionic Liquids for Gas Separations. *Industrial & Engineering Chemistry Research*, **2012**, 51, 11530-11537	3.9	37
81	Stabilizing gold clusters by heterostructured transition-metal oxide-mesoporous silica supports for enhanced catalytic activities for CO oxidation. *Chemical Communications*, **2012**, 48, 11413-5	5.8	72
80	Graphitic mesoporous carbon as a support of promoted Rh catalysts for hydrogenation of carbon monoxide to ethanol. *Carbon*, **2012**, 50, 1574-1582	10.4	34
79	Understanding controls on interfacial wetting at epitaxial graphene: Experiment and theory. *Physical Review B*, **2012**, 85,	3.3	85
78	B80 and B101-103 clusters: remarkable stability of the core-shell structures established by validated density functionals. *Journal of Chemical Physics*, **2012**, 136, 074302	3.9	131
77	Hollow polyhedral structures in small gold-sulfide clusters. *ACS Nano*, **2011**, 5, 1441-9	16.7	32
76	Physicochemical properties of imidazolium-derived ionic liquids with different C-2 substitutions. *Physical Chemistry Chemical Physics*, **2011**, 13, 21503-10	3.6	46
75	Oscillation of capacitance inside nanopores. *Nano Letters*, **2011**, 11, 5373-7	11.5	240

74	Functionalizing porous aromatic frameworks with polar organic groups for high-capacity and selective CO2 separation: a molecular simulation study. *Langmuir*, **2011**, 27, 3451-60	4	116
73	Interaction of Gold Clusters with a Hydroxylated Surface. *Journal of Physical Chemistry Letters*, **2011**, 2, 1211-5	6.4	37
72	Effect of Pore Topology and Accessibility on Gas Adsorption Capacity in Zeolitic Imidazolate Frameworks: Bringing Molecular Simulation Close to Experiment. *Journal of Physical Chemistry C*, **2011**, 115, 8126-8135	3.8	44
71	Interstaple dithiol cross-linking in Au25(SR)18 nanomolecules: a combined mass spectrometric and computational study. *Journal of the American Chemical Society*, **2011**, 133, 20258-66	16.4	71
70	Understanding the high solubility of CO2 in an ionic liquid with the tetracyanoborate anion. *Journal of Physical Chemistry B*, **2011**, 115, 9789-94	3.4	116
69	A classical density functional theory for interfacial layering of ionic liquids. *Soft Matter*, **2011**, 7, 11222	3.6	143
68	Accurate static and dynamic properties of liquid electrolytes for Li-ion batteries from ab initio molecular dynamics. *Journal of Physical Chemistry B*, **2011**, 115, 3085-90	3.4	104
67	Theoretical Insights into the Structures of Graphene Oxide and Its Chemical Conversions Between Graphene. *Journal of Computational and Theoretical Nanoscience*, **2011**, 8, 2406-2422	0.3	28
66	Tuning the Basicity of Ionic Liquids for Equimolar CO2 Capture. *Angewandte Chemie*, **2011**, 123, 5020-5024	3.6	99
65	Tuning the basicity of ionic liquids for equimolar CO2 capture. *Angewandte Chemie - International Edition*, **2011**, 50, 4918-22	16.4	517
64	Staple fitness: a concept to understand and predict the structures of thiolated gold nanoclusters. *Chemistry - A European Journal*, **2011**, 17, 12289-93	4.8	41
63	The role of low-coordinate oxygen on Co3O4(110) in catalytic CO oxidation. *Physical Chemistry Chemical Physics*, **2011**, 13, 978-84	3.6	106
62	Open-shell singlet character of stable derivatives of nonacene, hexacene and teranthene. *Organic Letters*, **2011**, 13, 3316-9	6.2	33
61	Electrochemical windows of sulfone-based electrolytes for high-voltage Li-ion batteries. *Journal of Physical Chemistry B*, **2011**, 115, 12120-5	3.4	94
60	Density functional theory for differential capacitance of planar electric double layers in ionic liquids. *Chemical Physics Letters*, **2011**, 504, 153-158	2.5	112
59	Au40: A large tetrahedral magic cluster. *Physical Review B*, **2011**, 84,	3.3	48
58	Computational investigation of reactive to nonreactive capture of carbon dioxide by oxygen-containing Lewis bases. *Journal of Physical Chemistry A*, **2010**, 114, 11761-7	2.8	50
57	Sequential Observation of AgnS4 (1 h 7) Gas Phase Clusters in MS/MS and Prediction of Their Structures. *Journal of Physical Chemistry Letters*, **2010**, 1, 1423-1427	6.4	28

56	Properties of π-Electrons in Graphene Nanoribbons and Nanographenes **2010**, 433-461		1
55	On the Structure of a Thiolated Gold Cluster: Au44(SR)28? *Journal of Physical Chemistry C*, **2010**, 114, 15883-15889	3.8	53
54	Gold sulfide nanoclusters: a unique core-in-cage structure. *Chemistry - A European Journal*, **2010**, 16, 4999-5003	5.8	33
53	Carbon Dioxide Capture by Superbase-Derived Protic Ionic Liquids. *Angewandte Chemie*, **2010**, 122, 6114-6117	3.6	112
52	Carbon dioxide capture by superbase-derived protic ionic liquids. *Angewandte Chemie - International Edition*, **2010**, 49, 5978-81	16.4	383
51	Magnetic doping of a thiolated-gold superatom: First-principles density functional theory calculations. *Physical Review B*, **2009**, 80,	3.3	60
50	Au adatom-linked CH3S-Au-SCH3 complexes on Au(1 1 1). *Chemical Physics Letters*, **2009**, 477, 90-94	2.5	10
49	From trans-polyacetylene to zigzag-edged graphene nanoribbons. *Chemical Physics Letters*, **2009**, 483, 120-123	2.5	23
48	Oxidation unzipping of stable nanographenes into joint spin-rich fragments. *Journal of the American Chemical Society*, **2009**, 131, 9663-9	16.4	44
47	Porous graphene as the ultimate membrane for gas separation. *Nano Letters*, **2009**, 9, 4019-24	11.5	733
46	Steric effects in the reaction of aryl radicals on surfaces. *Langmuir*, **2009**, 25, 286-93	4	103
45	Diffusion of the Linear CH3S-Au-SCH3 Complex on Au(111) from First Principles. *Journal of Physical Chemistry C*, **2009**, 113, 3763-3766	3.8	22
44	Constructing Gold(I) Thiolate Oligomers and Polymers on Au(111) Based on the Linear S-Au-S Geometry. *Journal of Physical Chemistry C*, **2009**, 113, 7838-7842	3.8	18
43	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
42	Thiolated gold nanowires: metallic versus semiconducting. *ACS Nano*, **2009**, 3, 2351-7	16.7	52
41	What Protects the Core When the Thiolated Au Cluster is Extremely Small?. *Journal of Physical Chemistry C*, **2009**, 113, 16983-16987	3.8	81
40	First principles study of the graphene/Ru(0001) interface. *Journal of Chemical Physics*, **2009**, 130, 074705	3.9	99
39	From superatomic Au25(SR)18(-) to superatomic M@Au24(SR)18(q) core-shell clusters. *Inorganic Chemistry*, **2009**, 48, 2720-2	5.1	153

38	The Smallest Thiolated Gold Superatom Complexes. *Journal of Physical Chemistry C*, **2009**, 113, 17291-17295	3.8	79
37	Cis-trans conversion of the CH3S-Au-SCH3 complex on Au(111). *Physical Chemistry Chemical Physics*, **2009**, 11, 8601-5	3.6	20
36	Spin States of Zigzag-Edged Möbius Graphene Nanoribbons from First Principles. *Journal of Physical Chemistry C*, **2008**, 112, 5348-5351	3.8	25
35	Advanced Liquid Membranes Based on Novel Ionic Liquids for Selective Separation of Olefin/Paraffin via Olefin-Facilitated Transport. *Industrial & Engineering Chemistry Research*, **2008**, 47, 881-888	3.9	85
34	Surface Modification of Ordered Mesoporous Carbons via 1,3-Dipolar Cycloaddition of Azomethine Ylides. *Chemistry of Materials*, **2008**, 20, 4800-4802	9.6	30
33	Hydrogen-Bonded Helices for Anion Binding and Separation. *Crystal Growth and Design*, **2008**, 8, 1909-1915	3.9	49
32	The "staple" motif: a key to stability of thiolate-protected gold nanoclusters. *Journal of the American Chemical Society*, **2008**, 130, 2777-9	16.4	217
31	Electronic ground state of higher acenes. *Journal of Physical Chemistry A*, **2008**, 112, 332-5	2.8	216
30	In Search of a Structural Model for a Thiolate-protected Au38 Cluster. *Journal of Physical Chemistry C*, **2008**, 112, 13905-13910	3.8	62
29	First principles molecular dynamics simulation of a task-specific ionic liquid based on silver-olefin complex: atomistic insights into a separation process. *Journal of Physical Chemistry B*, **2008**, 112, 10202-6	3.4	23
28	New insight into carbon-nanotube electronic-structure selectivity. *Small*, **2008**, 4, 2035-42	11	20
27	Sulfate recognition by persistent crystalline capsules with rigidified hydrogen-bonding cavities. *Angewandte Chemie - International Edition*, **2008**, 47, 1866-70	16.4	175
26	Circumacenes versus periacenes: HOMO–LUMO gap and transition from nonmagnetic to magnetic ground state with size. *Chemical Physics Letters*, **2008**, 466, 72-75	2.5	94
25	Open-shell singlet character of cyclacenes and short zigzag nanotubes. *Organic Letters*, **2007**, 9, 5449-52	6.2	135
24	First principles study of magnetism in nanographenes. *Journal of Chemical Physics*, **2007**, 127, 124703	3.9	178
23	Structure, magnetism, and adhesion at Cr/Fe interfaces from density functional theory. *Surface Science*, **2007**, 601, 699-705	1.8	26
22	Unique chemical reactivity of a graphene nanoribbon's zigzag edge. *Journal of Chemical Physics*, **2007**, 126, 134701	3.9	380
21	Olefin adsorption on silica-supported silver salts--a DFT study. *Langmuir*, **2006**, 22, 5716-22	4	20

20	Structure and bonding between an aryl group and metal surfaces. *Journal of the American Chemical Society*, **2006**, 128, 6030-1	16.4	125
19	How do aryl groups attach to a graphene sheet?. *Journal of Physical Chemistry B*, **2006**, 110, 23628-32	3.4	179
18	Prediction of a highly activated state of CO adsorbed on an Al/Fe(100) bimetallic surface. *Journal of Physical Chemistry B*, **2006**, 110, 22213-9	3.4	13
17	Effects of alloying on the chemistry of CO and H2S on Fe surfaces. *Journal of Physical Chemistry B*, **2005**, 109, 20469-78	3.4	22
16	First principles study of H2S adsorption and dissociation on Fe(110). *Surface Science*, **2005**, 583, 60-68	1.8	68
15	Prediction of strong adhesion at the MoSi2/Fe interface. *Acta Materialia*, **2005**, 53, 4489-4496	8.4	27
14	Adsorption and dissociation of CO on Fe(1 1 0) from first principles. *Surface Science*, **2004**, 570, 167-177	1.8	108
13	First principles assessment of ideal fracture energies of materials with mobile impurities: implications for hydrogen embrittlement of metals. *Acta Materialia*, **2004**, 52, 4801-4807	8.4	162
12	Adsorption, Diffusion, and Dissociation of H2S on Fe(100) from First Principles. *Journal of Physical Chemistry B*, **2004**, 108, 19140-19145	3.4	92
11	Adsorption and diffusion energetics of hydrogen atoms on Fe(110) from first principles. *Surface Science*, **2003**, 547, 85-98	1.8	148
10	Dispersion of Na2CO3 on γ-Al2O3 and the threshold effect in flue-gas desulfurization. *Fuel*, **2002**, 81, 1565-1568	7.1	14
9	Investigation of the Structure of γ-Al2O3-Supported MgO by Surface Extended Energy Loss Fine Structure. *Journal of Physical Chemistry A*, **2002**, 106, 2815-2819	2.8	8
8	Structure and basicity of γ-Al2O3-supported MgO and its application to mercaptan oxidation. *Applied Catalysis A: General*, **2001**, 219, 69-78	5.1	55
7	Preparation of ZrO2-supported MgO with high surface area and its use in mercaptan oxidation of jet fuel. *Applied Catalysis A: General*, **2000**, 201, 169-176	5.1	38
6	Dispersion of cobalt (II) phthalocyaninetetrasulfonate on active carbon. *Applied Catalysis A: General*, **2000**, 192, 1-8	5.1	20
5	Monolayer dispersion of MoO3, NiO and their precursors on γ-Al2O3. *Applied Catalysis A: General*, **1999**, 188, 201-209	5.1	64
4	Mechanism for Acetone and Crotonaldehyde Production during Steam Reforming of Ethanol over La0.7Sr0.3MnO3− Perovskite: Evidence for a Shared C4 Aldol Addition Intermediate. *ACS Catalysis*,4358-4374	13.1	0
3	Single Atoms Anchored in Hexagonal Boron Nitride for Propane Dehydrogenation from First Principles. *ChemCatChem*,	5.2	2

2	Ionic liquids for carbon capture. *MRS Bulletin*,	3.2	2
1	Molecular Dynamics Simulations of U(III) and U(IV) in Molten Chlorides. *ACS Symposium Series*,365-386	0.4	1