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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Porous graphene as the ultimate membrane for gas separation. <i>Nano Letters</i> , 2009 , 9, 4019-24	11.5	733
360	Tuning the basicity of ionic liquids for equimolar CO ₂ capture. <i>Angewandte Chemie - International Edition</i> , 2011 , 50, 4918-22	16.4	517
359	Mechanism of Hydrogen Evolution Reaction on 1T-MoS ₂ from First Principles. <i>ACS Catalysis</i> , 2016 , 6, 4953-4961	13.1	489
358	Identification of a highly luminescent Au ₂₂ (SG) ₁₈ nanocluster. <i>Journal of the American Chemical Society</i> , 2014 , 136, 1246-9	16.4	436
357	Pseudocapacitance: From Fundamental Understanding to High Power Energy Storage Materials. <i>Chemical Reviews</i> , 2020 , 120, 6738-6782	68.1	402
356	Monoplatinum doping of gold nanoclusters and catalytic application. <i>Journal of the American Chemical Society</i> , 2012 , 134, 16159-62	16.4	383
355	Carbon dioxide capture by superbase-derived protic ionic liquids. <i>Angewandte Chemie - International Edition</i> , 2010 , 49, 5978-81	16.4	383
354	Unique chemical reactivity of a graphene nanoribbon's zigzag edge. <i>Journal of Chemical Physics</i> , 2007 , 126, 134701	3.9	380
353	Nickel sulfides for electrocatalytic hydrogen evolution under alkaline conditions: a case study of crystalline NiS, NiS ₂ , and Ni ₃ S ₂ nanoparticles. <i>Catalysis Science and Technology</i> , 2016 , 6, 1077-1084	5.5	330
352	Ag ₂₉ (BDT) ₁₂ (TPP) ₄ : A Tetravalent Nanocluster. <i>Journal of the American Chemical Society</i> , 2015 , 137, 11970-5	16.4	284
351	Toward understanding the growth mechanism: tracing all stable intermediate species from reduction of Au(I)-thiolate complexes to evolution of Au ⁰ nanoclusters. <i>Journal of the American Chemical Society</i> , 2014 , 136, 10577-80	16.4	255
350	Oscillation of capacitance inside nanopores. <i>Nano Letters</i> , 2011 , 11, 5373-7	11.5	240
349	The "staple" motif: a key to stability of thiolate-protected gold nanoclusters. <i>Journal of the American Chemical Society</i> , 2008 , 130, 2777-9	16.4	217
348	Electronic ground state of higher acenes. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 332-5	2.8	216
347	Thiolate ligands as a double-edged sword for CO oxidation on CeO ₂ supported Au ₂₅ (SCH ₂ CH ₂ Ph) ₁₈ nanoclusters. <i>Journal of the American Chemical Society</i> , 2014 , 136, 6111-22	16.4	215
346	Multi-Molar Absorption of CO ₂ by the Activation of Carboxylate Groups in Amino Acid Ionic Liquids. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 7166-70	16.4	212
345	Stabilization and Band-Gap Tuning of the 1T-MoS ₂ Monolayer by Covalent Functionalization. <i>Chemistry of Materials</i> , 2015 , 27, 3743-3748	9.6	211

344	Isomerism in Au ₂₈ (SR) ₂₀ Nanocluster and Stable Structures. <i>Journal of the American Chemical Society</i> , 2016 , 138, 1482-5	16.4	202
343	A molecule-like PtAu(SCH) nanocluster as an electrocatalyst for hydrogen production. <i>Nature Communications</i> , 2017 , 8, 14723	17.4	196
342	How do aryl groups attach to a graphene sheet?. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 23628-32	3.4	179
341	Understanding seed-mediated growth of gold nanoclusters at molecular level. <i>Nature Communications</i> , 2017 , 8, 927	17.4	178
340	First principles study of magnetism in nanographenes. <i>Journal of Chemical Physics</i> , 2007 , 127, 124703	3.9	178
339	Golden single-atomic-site platinum electrocatalysts. <i>Nature Materials</i> , 2018 , 17, 1033-1039	27	177
338	Au ₁₉ nanocluster featuring a V-shaped alkynyl-gold motif. <i>Journal of the American Chemical Society</i> , 2015 , 137, 652-5	16.4	176
337	Sulfate recognition by persistent crystalline capsules with rigidified hydrogen-bonding cavities. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 1866-70	16.4	175
336	Lattice-Hydride Mechanism in Electrocatalytic CO Reduction by Structurally Precise Copper-Hydride Nanoclusters. <i>Journal of the American Chemical Society</i> , 2017 , 139, 9728-9736	16.4	164
335	First principles assessment of ideal fracture energies of materials with mobile impurities: implications for hydrogen embrittlement of metals. <i>Acta Materialia</i> , 2004 , 52, 4801-4807	8.4	162
334	Insights into Interfaces, Stability, Electronic Properties, and Catalytic Activities of Atomically Precise Metal Nanoclusters from First Principles. <i>Accounts of Chemical Research</i> , 2018 , 51, 2793-2802	24.3	156
333	The expanding universe of thiolated gold nanoclusters and beyond. <i>Nanoscale</i> , 2013 , 5, 7149-60	7.7	153
332	From superatomic Au ₂₅ (SR) ₁₈ (-) to superatomic M@Au ₂₄ (SR) ₁₈ (q) core-shell clusters. <i>Inorganic Chemistry</i> , 2009 , 48, 2720-2	5.1	153
331	Universal Surface Engineering of Transition Metals for Superior Electrocatalytic Hydrogen Evolution in Neutral Water. <i>Journal of the American Chemical Society</i> , 2017 , 139, 12283-12290	16.4	151
330	Solvent Effect on the Pore-Size Dependence of an Organic Electrolyte Supercapacitor. <i>Journal of Physical Chemistry Letters</i> , 2012 , 3, 1727-31	6.4	151
329	Adsorption and diffusion energetics of hydrogen atoms on Fe(110) from first principles. <i>Surface Science</i> , 2003 , 547, 85-98	1.8	148
328	Interconversion between Superatomic 6-Electron and 8-Electron Configurations of M@Au(SR) _n Clusters (M = Pd, Pt). <i>Journal of the American Chemical Society</i> , 2015 , 137, 10833-40	16.4	146
327	A classical density functional theory for interfacial layering of ionic liquids. <i>Soft Matter</i> , 2011 , 7, 11222	3.6	143

- 326 Single rhodium atoms anchored in micropores for efficient transformation of methane under mild conditions. *Nature Communications*, **2018**, 9, 1231 17.4 140
- 325 Quantum mechanical basis for kinetic diameters of small gaseous molecules. *Journal of Physical Chemistry A*, **2014**, 118, 1150-4 2.8 140
- 324 Open-shell singlet character of cyclacenes and short zigzag nanotubes. *Organic Letters*, **2007**, 9, 5449-526.2 135
- 323 Understanding the MXene Pseudocapitance. *Journal of Physical Chemistry Letters*, **2018**, 9, 1223-1228 6.4 133
- 322 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
- 321 Structure and bonding between an aryl group and metal surfaces. *Journal of the American Chemical Society*, **2006**, 128, 6030-1 16.4 125
- 320 Computational Insights into Materials and Interfaces for Capacitive Energy Storage. *Advanced Science*, **2017**, 4, 1700059 13.6 122
- 319 Gold nanowired: a linear (Au₂₅)(n) polymer from Au₂₅ molecular clusters. *ACS Nano*, **2014**, 8, 8505-12 16.7 122
- 318 Insights into CO₂/N₂ separation through nanoporous graphene from molecular dynamics. *Nanoscale*, **2013**, 5, 9984-7 7.7 120
- 317 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
- 316 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
- 315 Alkynyl-protected Au₂₃ nanocluster: a 12-electron system. *Angewandte Chemie - International Edition*, **2015**, 54, 5977-80 16.4 114
- 314 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
- 313 Density functional theory for differential capacitance of planar electric double layers in ionic liquids. *Chemical Physics Letters*, **2011**, 504, 153-158 2.5 112
- 312 Carbon Dioxide Capture by Superbase-Derived Protic Ionic Liquids. *Angewandte Chemie*, **2010**, 122, 6114-6117 13.6 112
- 311 Size Dependence of Atomically Precise Gold Nanoclusters in Chemoselective Hydrogenation and Active Site Structure. *ACS Catalysis*, **2014**, 4, 2463-2469 13.1 108
- 310 The strategies for improving carbon dioxide chemisorption by functionalized ionic liquids. *RSC Advances*, **2013**, 3, 15518 3.7 108
- 309 Adsorption and dissociation of CO on Fe(1 1 0) from first principles. *Surface Science*, **2004**, 570, 167-177 1.8 108

308	Enhancing the Capacitive Performance of Electric Double-Layer Capacitors with Ionic Liquid Mixtures. <i>ACS Energy Letters</i> , 2016 , 1, 21-26	20.1	107
307	The role of low-coordinate oxygen on Co ₃ O ₄ (110) in catalytic CO oxidation. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 978-84	3.6	106
306	Curvature Effect on the Capacitance of Electric Double Layers at Ionic Liquid/Onion-Like Carbon Interfaces. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 1058-63	6.4	104
305	Accurate static and dynamic properties of liquid electrolytes for Li-ion batteries from ab initio molecular dynamics. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 3085-90	3.4	104
304	Steric effects in the reaction of aryl radicals on surfaces. <i>Langmuir</i> , 2009 , 25, 286-93	4	103
303	Selective deposition of Ru nanoparticles on TiSi ₃ nanonet and its utilization for LiO ₂ formation and decomposition. <i>Journal of the American Chemical Society</i> , 2014 , 136, 8903-6	16.4	100
302	Precise control of alloying sites of bimetallic nanoclusters via surface motif exchange reaction. <i>Nature Communications</i> , 2017 , 8, 1555	17.4	100
301	Superatomic Orbitals under Spin-Orbit Coupling. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 3286-9	6.4	99
300	Tuning the Basicity of Ionic Liquids for Equimolar CO ₂ Capture. <i>Angewandte Chemie</i> , 2011 , 123, 5020-5024	3.6	99
299	First principles study of the graphene/Ru(0001) interface. <i>Journal of Chemical Physics</i> , 2009 , 130, 074705	5.9	99
298	Oxide-supported atomically precise gold nanocluster for catalyzing Sonogashira cross-coupling. <i>Journal of Catalysis</i> , 2013 , 306, 177-183	7.3	97
297	High CO ₂ solubility, permeability and selectivity in ionic liquids with the tetracyanoborate anion. <i>RSC Advances</i> , 2012 , 2, 11813	3.7	96
296	Microscopic Insights into the Electrochemical Behavior of Nonaqueous Electrolytes in Electric Double-Layer Capacitors. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 1260-7	6.4	95
295	Solid-Electrolyte Interphase Formation and Electrolyte Reduction at Li-Ion Battery Graphite Anodes: Insights from First-Principles Molecular Dynamics. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 24476-24481	3.8	94
294	Electrochemical windows of sulfone-based electrolytes for high-voltage Li-ion batteries. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 12120-5	3.4	94
293	Circumacenes versus periacenes: HOMO-LUMO gap and transition from nonmagnetic to magnetic ground state with size. <i>Chemical Physics Letters</i> , 2008 , 466, 72-75	2.5	94
292	Quantum Effects on the Capacitance of Graphene-Based Electrodes. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 22297-22303	3.8	92
291	Adsorption, Diffusion, and Dissociation of H ₂ S on Fe(100) from First Principles. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 19140-19145	3.4	92

290	Electrode materialIonic liquid coupling for electrochemical energy storage. <i>Nature Reviews Materials</i> , 2020 , 5, 787-808	73.3	89
289	Simulating the initial stage of phenolic resin carbonization via the ReaxFF reactive force field. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 6891-4	2.8	85
288	Understanding controls on interfacial wetting at epitaxial graphene: Experiment and theory. <i>Physical Review B</i> , 2012 , 85,	3.3	85
287	Advanced Liquid Membranes Based on Novel Ionic Liquids for Selective Separation of Olefin/Paraffin via Olefin-Facilitated Transport. <i>Industrial & Engineering Chemistry Research</i> , 2008 , 47, 881-888	3.9	85
286	Ion-Gated Gas Separation through Porous Graphene. <i>Nano Letters</i> , 2017 , 17, 1802-1807	11.5	84
285	Enhancing graphene capacitance by nitrogen: effects of doping configuration and concentration. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 4668-74	3.6	84
284	What Protects the Core When the Thiolated Au Cluster is Extremely Small?. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 16983-16987	3.8	81
283	Atomically Precise Bimetallic AuCu Nanocluster with an Icosidodecahedral Cu Shell and an Alkynyl-Cu Interface. <i>Journal of the American Chemical Society</i> , 2017 , 139, 9451-9454	16.4	79
282	The Smallest Thiolated Gold Superatom Complexes. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 17291-17295	13.85	79
281	Selectivity trend of gas separation through nanoporous graphene. <i>Journal of Solid State Chemistry</i> , 2015 , 224, 2-6	3.3	77
280	Selective Charging Behavior in an Ionic Mixture Electrolyte-Supercapacitor System for Higher Energy and Power. <i>Journal of the American Chemical Society</i> , 2017 , 139, 18681-18687	16.4	76
279	Three-orders-of-magnitude variation of carrier lifetimes with crystal phase of gold nanoclusters. <i>Science</i> , 2019 , 364, 279-282	33.3	75
278	Revealing isoelectronic size conversion dynamics of metal nanoclusters by a noncrystallization approach. <i>Nature Communications</i> , 2018 , 9, 1979	17.4	75
277	Synthesis of Water-Soluble [Au(SR)] Using a Stoichiometric Amount of NaBH ₄ . <i>Journal of the American Chemical Society</i> , 2018 , 140, 11370-11377	16.4	72
276	Stabilizing gold clusters by heterostructured transition-metal oxide-mesoporous silica supports for enhanced catalytic activities for CO oxidation. <i>Chemical Communications</i> , 2012 , 48, 11413-5	5.8	72
275	Interstaple dithiol cross-linking in Au ₂₅ (SR) ₁₈ nanomolecules: a combined mass spectrometric and computational study. <i>Journal of the American Chemical Society</i> , 2011 , 133, 20258-66	16.4	71
274	Diphosphine-Protected Au Nanoclusters on Oxide Supports Are Active for Gas-Phase Catalysis without Ligand Removal. <i>Nano Letters</i> , 2016 , 16, 6560-6567	11.5	70
273	First principles study of H ₂ S adsorption and dissociation on Fe(110). <i>Surface Science</i> , 2005 , 583, 60-68	1.8	68

272	Computational Discovery and Design of MXenes for Energy Applications: Status, Successes, and Opportunities. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 24885-24905	9.5	65
271	Global minimization of gold clusters by combining neural network potentials and the basin-hopping method. <i>Nanoscale</i> , 2015 , 7, 14817-21	7.7	64
270	CoP for hydrogen evolution: implications from hydrogen adsorption. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 23864-71	3.6	64
269	Monolayer dispersion of MoO ₃ , NiO and their precursors on Al ₂ O ₃ . <i>Applied Catalysis A: General</i> , 1999 , 188, 201-209	5.1	64
268	Highly Efficient Carbon Monoxide Capture by Carbanion-Functionalized Ionic Liquids through C-Site Interactions. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 6843-6847	16.4	63
267	In Search of a Structural Model for a Thiolate-protected Au ₃₈ Cluster. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 13905-13910	3.8	62
266	CO ₂ Adsorption As a Flat-Lying, Tridentate Carbonate on CeO ₂ (100). <i>Journal of Physical Chemistry C</i> , 2014 , 118, 9042-9050	3.8	61
265	Oxidation potentials of functionalized sulfone solvents for high-voltage Li-ion batteries: a computational study. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 3235-8	3.4	60
264	Magnetic doping of a thiolated-gold superatom: First-principles density functional theory calculations. <i>Physical Review B</i> , 2009 , 80,	3.3	60
263	Unusual effects of solvent polarity on capacitance for organic electrolytes in a nanoporous electrode. <i>Nanoscale</i> , 2014 , 6, 5545-50	7.7	58
262	Windowed Carbon Nanotubes for Efficient CO ₂ Removal from Natural Gas. <i>Journal of Physical Chemistry Letters</i> , 2012 , 3, 3343-3347	6.4	57
261	A Generic Model for Electric Double Layers in Porous Electrodes. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 8704-8710	3.8	57
260	Effects of Metal-Doping on Hydrogen Evolution Reaction Catalyzed by MAu and MAu Nanoclusters (M = Pt, Pd). <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 44645-44653	9.5	57
259	Understanding Selective Hydrogenation of α -Unsaturated Ketones to Unsaturated Alcohols on the Au ₂₅ (SR) ₁₈ Cluster. <i>ACS Catalysis</i> , 2015 , 5, 6624-6629	13.1	56
258	Expanded Porphyrins as Two-Dimensional Porous Membranes for CO ₂ Separation. <i>ACS Applied Materials & Interfaces</i> , 2015 , 7, 13073-9	9.5	55
257	SO absorption in EmimCl-TEG deep eutectic solvents. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 15168-15173	9.6	55
256	Highly soluble alkoxide magnesium salts for rechargeable magnesium batteries. <i>Journal of Materials Chemistry A</i> , 2014 , 2, 581-584	13	55
255	Structure and basicity of Al ₂ O ₃ -supported MgO and its application to mercaptan oxidation. <i>Applied Catalysis A: General</i> , 2001 , 219, 69-78	5.1	55

- 254 Metallic Hydrogen in Atomically Precise Gold Nanoclusters. *Chemistry of Materials*, **2017**, 29, 4840-4847 9.6 54
- 253 Alkynyl-protected silver nanoclusters featuring an anticuboctahedral kernel. *Nanoscale*, **2017**, 9, 11405-11409 11.4 54
- 252 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
- 251 On the Structure of a Thiolated Gold Cluster: Au₄₄(SR)₂₈₂. *Journal of Physical Chemistry C*, **2010**, 114, 15883-15889 3.8 53
- 250 Porous liquid zeolites: hydrogen bonding-stabilized H-ZSM-5 in branched ionic liquids. *Nanoscale*, **2019**, 11, 1515-1519 7.7 52
- 249 Boron Supercapacitors. *ACS Energy Letters*, **2016**, 1, 1241-1246 20.1 52
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- 247 Thiolated gold nanowires: metallic versus semiconducting. *ACS Nano*, **2009**, 3, 2351-7 16.7 52
- 246 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
- 245 The surface structure of silver-coated gold nanocrystals and its influence on shape control. *Nature Communications*, **2015**, 6, 7664 17.4 50
- 244 The ligand effect on the isomer stability of Au₂₄(SR)₂₀ clusters. *Nanoscale*, **2015**, 7, 2225-9 7.7 50
- 243 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
- 242 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
- 241 Transforming Porous Organic Cages into Porous Ionic Liquids via a Supramolecular Complexation Strategy. *Angewandte Chemie - International Edition*, **2020**, 59, 2268-2272 16.4 50
- 240 General Structure-Reactivity Relationship for Oxygen on Transition-Metal Oxides. *Journal of Physical Chemistry Letters*, **2017**, 8, 2206-2211 6.4 49
- 239 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
- 238 Hydrogen-Bonded Helices for Anion Binding and Separation. *Crystal Growth and Design*, **2008**, 8, 1909-1915 3.5 49
- 237 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

236	Real Time Monitoring of the Dynamic Intracluster Diffusion of Single Gold Atoms into Silver Nanoclusters. <i>Journal of the American Chemical Society</i> , 2019 , 141, 18977-18983	16.4	48
235	Kinetic Charging Inversion in Ionic Liquid Electric Double Layers. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 2195-200	6.4	48
234	Au ₄₀ : A large tetrahedral magic cluster. <i>Physical Review B</i> , 2011 , 84,	3.3	48
233	Rational design and synthesis of a porous, task-specific polycarbazole for efficient CO ₂ capture. <i>Chemical Communications</i> , 2016 , 52, 4454-7	5.8	47
232	Computational Screening of MXene Electrodes for Pseudocapacitive Energy Storage. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 315-321	3.8	47
231	Comprehensive View of the Ligand-Gold Interface from First Principles. <i>Chemistry of Materials</i> , 2017 , 29, 6908-6915	9.6	46
230	Physicochemical properties of imidazolium-derived ionic liquids with different C-2 substitutions. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 21503-10	3.6	46
229	Insights into the PhC≡C/Au Interface. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 10804-10810	3.8	45
228	Solubility of gases in a common ionic liquid from molecular dynamics based free energy calculations. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 2719-25	3.4	44
227	Effect of Pore Topology and Accessibility on Gas Adsorption Capacity in Zeolitic-Imidazolate Frameworks: Bringing Molecular Simulation Close to Experiment. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 8126-8135	3.8	44
226	Oxidation unzipping of stable nanographenes into joint spin-rich fragments. <i>Journal of the American Chemical Society</i> , 2009 , 131, 9663-9	16.4	44
225	Alkynyl-Protected Au ₂₃ Nanocluster: A 12-Electron System. <i>Angewandte Chemie</i> , 2015 , 127, 6075-6078	3.6	43
224	Efficient Absorption of SO ₂ by Deep Eutectic Solvents Formed by Biobased Aprotic Organic Compound Succinonitrile and 1-Ethyl-3-methylimidazolium Chloride. <i>ACS Sustainable Chemistry and Engineering</i> , 2019 , 7, 9086-9091	8.3	42
223	A Poly(acrylonitrile)-Functionalized Porous Aromatic Framework Synthesized by Atom-Transfer Radical Polymerization for the Extraction of Uranium from Seawater. <i>Industrial & Engineering Chemistry Research</i> , 2016 , 55, 4125-4129	3.9	42
222	Stronger-than-Pt hydrogen adsorption in a Au ₂₂ nanocluster for the hydrogen evolution reaction. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 7532-7537	13	41
221	Staple fitness: a concept to understand and predict the structures of thiolated gold nanoclusters. <i>Chemistry - A European Journal</i> , 2011 , 17, 12289-93	4.8	41
220	Interface Engineering of Earth-Abundant Transition Metals Using Boron Nitride for Selective Electroreduction of CO. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 6694-6700	9.5	40
219	Low-temperature activation of methane on doped single atoms: descriptor and prediction. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 22909-22914	3.6	40

218	All-Carboxylate-Protected Superatomic Silver Nanocluster with an Unprecedented Rhombohedral Ag Core. <i>Journal of the American Chemical Society</i> , 2020 , 142, 16905-16909	16.4	40
217	First-Principles Insight into Electrocatalytic Reduction of CO ₂ to CH ₄ on a Copper Nanoparticle. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 11392-11398	3.8	39
216	Molecular Dynamics Simulation of Anion Effect on Solubility, Diffusivity, and Permeability of Carbon Dioxide in Ionic Liquids. <i>Industrial & Engineering Chemistry Research</i> , 2014 , 53, 10485-10490	3.9	39
215	Mechanochemical synthesis of pillar[5]quinone derived multi-microporous organic polymers for radioactive organic iodide capture and storage. <i>Nature Communications</i> , 2020 , 11, 1086	17.4	38
214	Thiolate-Protected Trimetallic AuAgPd and AuAgPt Alloy Clusters with Controlled Chemical Composition and Metal Positions. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 2590-2594	6.4	38
213	Identify the Removable Substructure in Carbon Activation. <i>Chemistry of Materials</i> , 2017 , 29, 7288-7295	9.6	38
212	Nitrogen-Doped Mesoporous Carbon for Carbon Capture [A Molecular Simulation Study. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 7106-7110	3.8	38
211	Preparation of ZrO ₂ -supported MgO with high surface area and its use in mercaptan oxidation of jet fuel. <i>Applied Catalysis A: General</i> , 2000 , 201, 169-176	5.1	38
210	Dopant-Dependent Electronic Structures Observed for MAu(SCH) Clusters (M = Pt, Pd). <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 982-989	6.4	37
209	Time-dependent density functional theory for ion diffusion in electrochemical systems. <i>Journal of Physics Condensed Matter</i> , 2014 , 26, 284102	1.8	37
208	Synthesis and Characterization of Lithium Bis(fluoromalonato)borate for Lithium-Ion Battery Applications. <i>Advanced Energy Materials</i> , 2014 , 4, 1301368	21.8	37
207	Synthesis and Characterization of Thiazolium-Based Room Temperature Ionic Liquids for Gas Separations. <i>Industrial & Engineering Chemistry Research</i> , 2012 , 51, 11530-11537	3.9	37
206	Interaction of Gold Clusters with a Hydroxylated Surface. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 1211-5	6.4	37
205	Understanding the Impact of Surface Reconstruction of Perovskite Catalysts on CH ₄ Activation and Combustion. <i>ACS Catalysis</i> , 2018 , 8, 10306-10315	13.1	36
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