Yousung Jung

List of Publications by Year in Descending Order

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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.

202 papers	17,932 citations	63 h-index	132 g-index
218 ext. papers	20,789 ext. citations	9.8 avg, IF	6.99 L-index

#	Paper	IF	Citations
202	An invertible crystallographic representation for general inverse design of inorganic crystals with targeted properties. *Matter*, **2022**, 5, 314-335	12.7	4
201	Engineering vacancy and hydrophobicity of two-dimensional TaTe for efficient and stable electrocatalytic N reduction.. *Innovation(China)*, **2022**, 3, 100190	17.8	5
200	Recent progress in computational discovery of Heusler alloys. *Bulletin of the Korean Chemical Society*, **2022**, 43, 484-491	1.2	0
199	Single atom and defect engineering of CuO for efficient electrochemical reduction of CO 2 to C 2 H 4. *SmartMat*, **2022**, 3, 194-205	22.8	1
198	Automated exploitation of the big configuration space of large adsorbates on transition metals reveals chemistry feasibility.. *Nature Communications*, **2022**, 13, 2087	17.4	1
197	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
196	Enhanced electrochemical CO2 reduction to ethylene over CuO by synergistically tuning oxygen vacancies and metal doping. *Cell Reports Physical Science*, **2021**, 2, 100356	6.1	15
195	High Facets on Nanowrinkled Cu via Chemical Vapor Deposition Graphene Growth for Efficient CO2 Reduction into Ethanol. *ACS Catalysis*, **2021**, 11, 5658-5665	13.1	13
194	Pd Pb Nanosponges for Selective Conversion of Furfural to Furfuryl Alcohol under Mild Condition.. *Small Methods*, **2021**, 5, e2100400	12.8	1
193	Understanding potential-dependent competition between electrocatalytic dinitrogen and proton reduction reactions. *Nature Communications*, **2021**, 12, 4353	17.4	22
192	Electrochemical ammonia synthesis: Mechanistic understanding and catalyst design. *CheM*, **2021**, 7, 1708-1754	16.2	70
191	Shifting the scaling relations of single-atom catalysts for facile methane activation by tuning the coordination number. *Chemical Science*, **2021**, 12, 3551-3557	9.4	3
190	Predicting potentially hazardous chemical reactions using an explainable neural network. *Chemical Science*, **2021**, 12, 11028-11037	9.4	0
189	Theoretical Study on the Degree of CO Activation in CO-Coordinated Ni(0) Complexes. *ACS Omega*, **2021**, 6, 7646-7654	3.9	2
188	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
187	Deep Retrosynthetic Reaction Prediction using Local Reactivity and Global Attention. *Jacs Au*, **2021**, 1, 1612-1620		6
186	Vertical-crystalline Fe-doped Ni oxyhydroxides for highly active and stable oxygen evolution reaction. *Matter*, **2021**,	12.7	4

185	Controlling hot electron flux and catalytic selectivity with nanoscale metal-oxide interfaces. *Nature Communications*, **2021**, 12, 40	17.4	7
184	Surface overgrowth on gold nanoparticles modulating high-energy facets for efficient electrochemical CO reduction. *Nanoscale*, **2021**, 13, 14346-14353	7.7	0
183	Highly stable two-dimensional bismuth metal-organic frameworks for efficient electrochemical reduction of CO2. *Applied Catalysis B: Environmental*, **2020**, 277, 119241	21.8	53
182	Progress in Computational and Machine-Learning Methods for Heterogeneous Small-Molecule Activation. *Advanced Materials*, **2020**, 32, e1907865	24	23
181	Interaction Mediator Assisted Synthesis of Mesoporous Molybdenum Carbide: Mo-Valence State Adjustment for Optimizing Hydrogen Evolution. *ACS Nano*, **2020**, 14, 4988-4999	16.7	50
180	Uncertainty-Quantified Hybrid Machine Learning/Density Functional Theory High Throughput Screening Method for Crystals. *Journal of Chemical Information and Modeling*, **2020**, 60, 1996-2003	6.1	12
179	Practical Deep-Learning Representation for Fast Heterogeneous Catalyst Screening. *Journal of Physical Chemistry Letters*, **2020**, 11, 3185-3191	6.4	29
178	Selective electrocatalysis imparted by metal□nsulator transition for durability enhancement of automotive fuel cells. *Nature Catalysis*, **2020**, 3, 639-648	36.5	32
177	Machine-enabled inverse design of inorganic solid materials: promises and challenges. *Chemical Science*, **2020**, 11, 4871-4881	9.4	42
176	Tunable sieving of small gas molecules using horizontal graphene oxide membrane. *Journal of Membrane Science*, **2020**, 610, 118178	9.6	9
175	Towards stable Na-rich layered transition metal oxides for high energy density sodium-ion batteries. *Energy Storage Materials*, **2020**, 25, 62-69	19.4	17
174	Charge-transfer descriptor for the cycle performance of □Li2MO3 cathodes: role of oxygen dimers. *Journal of Materials Chemistry A*, **2020**, 8, 2663-2671	13	5
173	Aqueous lithium-ion batteries with niobium tungsten oxide anodes for superior volumetric and rate capability. *Energy Storage Materials*, **2020**, 27, 506-513	19.4	20
172	Activation of Ni Particles into Single Ni□N Atoms for Efficient Electrochemical Reduction of CO2. *Advanced Energy Materials*, **2020**, 10, 1903068	21.8	111
171	Reduced graphene oxides with engineered defects enable efficient electrochemical reduction of dinitrogen to ammonia in wide pH range. *Nano Energy*, **2020**, 68, 104323	17.1	43
170	Surface-engineered oxidized two-dimensional Sb for efficient visible light-driven N2 fixation. *Nano Energy*, **2020**, 78, 105368	17.1	21
169	Longitudinal unzipping of 2D transition metal dichalcogenides. *Nature Communications*, **2020**, 11, 5032	17.4	7
168	Highly durable fuel cell catalysts using crosslinkable block copolymer-based carbon supports with ultralow Pt loadings. *Energy and Environmental Science*, **2020**, 13, 4921-4929	35.4	28

167	Generative Adversarial Networks for Crystal Structure Prediction. *ACS Central Science*, **2020**, 6, 1412-1420	16.8	35
166	Single yttrium sites on carbon-coated TiO for efficient electrocatalytic N reduction. *Chemical Communications*, **2020**, 56, 10910-10913	5.8	15
165	Structure-Based Synthesizability Prediction of Crystals Using Partially Supervised Learning. *Journal of the American Chemical Society*, **2020**, 142, 18836-18843	16.4	19
164	Stabilization of Cu+ by tuning a CuO□eO2 interface for selective electrochemical CO2 reduction to ethylene. *Green Chemistry*, **2020**, 22, 6540-6546	10	34
163	Inverse Design of Solid-State Materials via a Continuous Representation. *Matter*, **2019**, 1, 1370-1384	12.7	99
162	Efficient visible-light driven N fixation over two-dimensional Sb/TiO composites. *Chemical Communications*, **2019**, 55, 7171-7174	5.8	31
161	Enhanced rate capability due to highly active Ta2O5 catalysts for lithium sulfur batteries. *Journal of Power Sources*, **2019**, 435, 226707	8.9	15
160	Mixed Transition Metal Oxide with Vacancy-Induced Lattice Distortion for Enhanced Catalytic Activity of Oxygen Evolution Reaction. *ACS Catalysis*, **2019**, 9, 7099-7108	13.1	52
159	Oxygen vacancy enables electrochemical N2 fixation over WO3 with tailored structure. *Nano Energy*, **2019**, 62, 869-875	17.1	94
158	Machine learning for renewable energy materials. *Journal of Materials Chemistry A*, **2019**, 7, 17096-17117	13	114
157	Ambient Stabilization of Few Layer Phosphorene via Noncovalent Functionalization with Surfactants: Systematic 2D NMR Characterization in Aqueous Dispersion. *Chemistry of Materials*, **2019**, 31, 2786-2794	9.6	30
156	High-yield production of few-layer boron nanosheets for efficient electrocatalytic N reduction. *Chemical Communications*, **2019**, 55, 4246-4249	5.8	71
155	Low-Dimensional Confined Ice Has the Electronic Signature of Liquid Water. *Journal of Physical Chemistry Letters*, **2019**, 10, 2008-2016	6.4	5
154	Intrinsic Relation between Hot Electron Flux and Catalytic Selectivity during Methanol Oxidation. *ACS Catalysis*, **2019**, 9, 8424-8432	13.1	6
153	Lattice Convolutional Neural Network Modeling of Adsorbate Coverage Effects. *Journal of Physical Chemistry C*, **2019**, 123, 18951-18959	3.8	16
152	Activated TiO2 with tuned vacancy for efficient electrochemical nitrogen reduction. *Applied Catalysis B: Environmental*, **2019**, 257, 117896	21.8	130
151	Hydrated Intercalation for High-Performance Aqueous Zinc Ion Batteries. *Advanced Energy Materials*, **2019**, 9, 1900083	21.8	158
150	Unveiling new stable manganese based photoanode materials via theoretical high-throughput screening and experiments. *Chemical Communications*, **2019**, 55, 13418-13421	5.8	9

149	Nitrogen Fixation by Ru Single-Atom Electrocatalytic Reduction. *CheM*, **2019**, 5, 204-214	16.2	501
148	Understanding the Effects of Au Morphology on CO2 Electrocatalysis. *Journal of Physical Chemistry C*, **2018**, 122, 4274-4280	3.8	29
147	Tungsten Carbide as a Highly Efficient Catalyst for Polysulfide Fragmentations in Li‒S Batteries. *Journal of Physical Chemistry C*, **2018**, 122, 7664-7669	3.8	31
146	pH-Dependent Conformations for Hyperbranched Poly(ethylenimine) from All-Atom Molecular Dynamics. *Macromolecules*, **2018**, 51, 2187-2194	5.5	11
145	Highly Efficient Catalytic Cyclic Carbonate Formation by Pyridyl Salicylimines. *ACS Applied Materials & Interfaces*, **2018**, 10, 9478-9484	9.5	64
144	Active learning with non- input features toward efficient CO reduction catalysts. *Chemical Science*, **2018**, 9, 5152-5159	9.4	42
143	Diamine-Functionalization of a Metal-Organic Framework Adsorbent for Superb Carbon Dioxide Adsorption and Desorption Properties. *ChemSusChem*, **2018**, 11, 1694-1707	8.3	30
142	A catalytic role of surface silanol groups in CO capture on the amine-anchored silica support. *Physical Chemistry Chemical Physics*, **2018**, 20, 12149-12156	3.6	9
141	Nanostructuring one-dimensional and amorphous lithium peroxide for high round-trip efficiency in lithium-oxygen batteries. *Nature Communications*, **2018**, 9, 680	17.4	50
140	Polyselenide Anchoring Using Transition-Metal Disulfides for Enhanced Lithium-Selenium Batteries. *Inorganic Chemistry*, **2018**, 57, 2149-2156	5.1	17
139	The Role of Adsorbed CN and Cl on an Au Electrode for Electrochemical CO2 Reduction. *ACS Catalysis*, **2018**, 8, 1178-1185	13.1	67
138	Infrared spectroscopy and density functional calculations on titanium-dinitrogen complexes. *Chemical Physics Letters*, **2018**, 698, 163-170	2.5	2
137	Origin of unusual spinel-to-layered phase transformation by crystal water. *Chemical Science*, **2018**, 9, 433-438	9.4	23
136	A local environment descriptor for machine-learned density functional theory at the generalized gradient approximation level. *Journal of Chemical Physics*, **2018**, 148, 241742	3.9	9
135	Tuning the Pd-catalyzed electroreduction of CO2 to CO with reduced overpotential. *Catalysis Science and Technology*, **2018**, 8, 3894-3900	5.5	20
134	Computational exploration of borophane-supported single transition metal atoms as potential oxygen reduction and evolution electrocatalysts. *Physical Chemistry Chemical Physics*, **2018**, 20, 21095-21104	3.6	39
133	Revealing the Role of Oxygen Debris and Functional Groups on the Water Flux and Molecular Separation of Graphene Oxide Membrane: A Combined Experimental and Theoretical Study. *Journal of Physical Chemistry C*, **2018**, 122, 17507-17517	3.8	22
132	Adsorbate-driven reactive interfacial Pt-NiO nanostructure formation on the PtNi(111) alloy surface. *Science Advances*, **2018**, 4, eaat3151	14.3	53

131	Ultralow Overpotential of Hydrogen Evolution Reaction using Fe-Doped Defective Graphene: A Density Functional Study. *ChemCatChem*, **2018**, 10, 4450-4455	5.2	10
130	Activating Transition Metal Dichalcogenides by Substitutional Nitrogen-Doping for Potential ORR Electrocatalysts. *ChemElectroChem*, **2018**, 5, 4029-4035	4.3	17
129	Boosting hot electron flux and catalytic activity at metal-oxide interfaces of PtCo bimetallic nanoparticles. *Nature Communications*, **2018**, 9, 2235	17.4	56
128	Doping palladium with tellurium for the highly selective electrocatalytic reduction of aqueous CO to CO. *Chemical Science*, **2018**, 9, 483-487	9.4	73
127	Carbon-supported Ni nanoparticles for efficient CO electroreduction. *Chemical Science*, **2018**, 9, 8775-8780	9.4	116
126	Studies on Catalytic Activity of Hydrogen Peroxide Generation according to Au Shell Thickness of Pd/Au Nanocubes. *ACS Applied Materials & Interfaces*, **2018**, 10, 38109-38116	9.5	22
125	Suppression of Hydrogen Evolution Reaction in Electrochemical N2 Reduction Using Single-Atom Catalysts: A Computational Guideline. *ACS Catalysis*, **2018**, 8, 7517-7525	13.1	333
124	Edge-Functionalized Graphene Nanoribbon Frameworks for the Capture and Separation of Greenhouse Gases. *Macromolecules*, **2017**, 50, 523-533	5.5	11
123	Heterogeneous Catalysis for Lithium–Sulfur Batteries: Enhanced Rate Performance by Promoting Polysulfide Fragmentations. *ACS Energy Letters*, **2017**, 2, 327-333	20.1	141
122	A Novel Fabrication of 3.6 nm High Graphene Nanochannels for Ultrafast Ion Transport. *Advanced Materials*, **2017**, 29, 1605854	24	15
121	EEWS 2016: Progress and Perspectives of Energy Science and Technology. *ACS Energy Letters*, **2017**, 2, 592-594	20.1	
120	Importance of Ligand Effects Breaking the Scaling Relation for Core–Shell Oxygen Reduction Catalysts. *ChemCatChem*, **2017**, 9, 3173-3179	5.2	21
119	Highly active and selective Au thin layer on Cu polycrystalline surface prepared by galvanic displacement for the electrochemical reduction of CO2 to CO. *Applied Catalysis B: Environmental*, **2017**, 213, 211-215	21.8	38
118	TiC- and TiN-Supported Single-Atom Catalysts for Dramatic Improvements in CO2 Electrochemical Reduction to CH4. *ACS Energy Letters*, **2017**, 2, 969-975	20.1	134
117	Artificial neural network for the configuration problem in solids. *Journal of Chemical Physics*, **2017**, 146, 064103	3.9	6
116	Stability, Molecular Sieving, and Ion Diffusion Selectivity of a Lamellar Membrane from Two-Dimensional Molybdenum Disulfide. *Nano Letters*, **2017**, 17, 2342-2348	11.5	103
115	Selective nitrogen capture by porous hybrid materials containing accessible transition metal ion sites. *Nature Materials*, **2017**, 16, 526-531	27	135
114	Probing surface oxide formations on SiO2-supported platinum nanocatalysts under CO oxidation. *RSC Advances*, **2017**, 7, 45003-45009	3.7	18

113	One dimensional building blocks for molecular separation: laminated graphitic nanoribbons. *Nanoscale*, **2017**, 9, 19114-19123	7.7	19
112	Balancing activity, stability and conductivity of nanoporous core-shell iridium/iridium oxide oxygen evolution catalysts. *Nature Communications*, **2017**, 8, 1449	17.4	168
111	Multilayer Two-Dimensional Water Structure Confined in MoS2. *Journal of Physical Chemistry C*, **2017**, 121, 16021-16028	3.8	23
110	Single-atom catalysts for CO electroreduction with significant activity and selectivity improvements. *Chemical Science*, **2017**, 8, 1090-1096	9.4	319
109	Tuning the Phase Stability of Sodium Metal Pyrophosphates for Synthesis of High Voltage Cathode Materials. *Chemistry of Materials*, **2016**, 28, 6724-6730	9.6	12
108	Bifunctional Interface of Au and Cu for Improved CO2 Electroreduction. *ACS Applied Materials & Interfaces*, **2016**, 8, 23022-7	9.5	67
107	Alcohol Dimer is Requisite to Form an Alkyl Oxonium Ion in the Proton Transfer of a Strong (Photo)Acid to Alcohol. *Chemistry - A European Journal*, **2016**, 22, 4340-4	4.8	12
106	Defect-Controlled Formation of Triclinic Na2 CoP2 O7 for 4 V Sodium-Ion Batteries. *Angewandte Chemie - International Edition*, **2016**, 55, 6662-6	16.4	55
105	Adsorption of Carbon Dioxide on Unsaturated Metal Sites in M2 (dobpdc) Frameworks with Exceptional Structural Stability and Relation between Lewis Acidity and Adsorption Enthalpy. *Chemistry - A European Journal*, **2016**, 22, 7444-51	4.8	25
104	Ti(N5)4 as a Potential Nitrogen-Rich Stable High-Energy Density Material. *Journal of Physical Chemistry A*, **2016**, 120, 4249-55	2.8	20
103	The critical size of hydrogen-bonded alcohol clusters as effective Brønsted bases in solutions. *Physical Chemistry Chemical Physics*, **2016**, 18, 24880-9	3.6	9
102	Optimal Activation of Porous Carbon for High Performance CO2 Capture. *ChemNanoMat*, **2016**, 2, 528-533	3.5	10
101	Porous cationic polymers: the impact of counteranions and charges on CO2 capture and conversion. *Chemical Communications*, **2016**, 52, 934-7	5.8	127
100	On the mechanism of high product selectivity for HCOOH using Pb in CO2 electroreduction. *Physical Chemistry Chemical Physics*, **2016**, 18, 9652-7	3.6	47
99	Alcohol Dimer is Requisite to Form an Alkyl Oxonium Ion in the Proton Transfer of a Strong (Photo)Acid to Alcohol. *Chemistry - A European Journal*, **2016**, 22, 4301-4301	4.8	1
98	Computational Analysis of Pressure-Dependent Optimal Pore Size for CO2 Capture with Graphitic Surfaces. *Journal of Physical Chemistry C*, **2016**, 120, 3978-3985	3.8	10
97	On the mechanism of electrochemical ammonia synthesis on the Ru catalyst. *Physical Chemistry Chemical Physics*, **2016**, 18, 9161-6	3.6	111
96	Defect-Controlled Formation of Triclinic Na2CoP2O7 for 4 V Sodium-Ion Batteries. *Angewandte Chemie*, **2016**, 128, 6774-6778	3.6	5

95	Unexpected solution phase formation of hollow PtSn alloy nanoparticles from Sn deposition on Pt dendritic structures. *CrystEngComm*, **2016**, 18, 6019-6023	3.3	4
94	A soft damping function for dispersion corrections with less overfitting. *Journal of Chemical Physics*, **2016**, 145, 174104	3.9	3
93	A potential role of a substrate as a base for the deprotonation pathway in Rh-catalysed C-H amination of heteroarenes: DFT insights. *Dalton Transactions*, **2016**, 45, 7980-5	4.3	12
92	Observation of the wrapping mechanism in amine carbon dioxide molecular interactions on heterogeneous sorbents. *Physical Chemistry Chemical Physics*, **2016**, 18, 14177-81	3.6	34
91	A perspective on the density matrix purification for linear scaling electronic structure calculations. *International Journal of Quantum Chemistry*, **2016**, 116, 563-568	2.1	5
90	Effects of boron oxidation state on electrocatalytic activity of carbons synthesized from CO2. *Journal of Materials Chemistry A*, **2015**, 3, 5843-5849	13	20
89	Active Sites of Au and Ag Nanoparticle Catalysts for CO2Electroreduction to CO. *ACS Catalysis*, **2015**, 5, 5089-5096	13.1	326
88	Critical Role of Crystal Water for a Layered Cathode Material in Sodium Ion Batteries. *Chemistry of Materials*, **2015**, 27, 3721-3725	9.6	142
87	Two-Dimensional Transition Metal Dichalcogenide Monolayers as Promising Sodium Ion Battery Anodes. *Journal of Physical Chemistry C*, **2015**, 119, 26374-26380	3.8	210
86	Mechanistic Study on C□ Bond Formation of a Nickel(I) Monocarbonyl Species with Alkyl Iodides: Experimental and Computational Investigations. *Organometallics*, **2015**, 34, 4305-4311	3.8	21
85	Selective Heterogeneous CO2 Electroreduction to Methanol. *ACS Catalysis*, **2015**, 5, 965-971	13.1	137
84	Analytical double-hybrid density functional based on the polynomial series expansion of adiabatic connection: a quadratic approximation. *Journal of Chemical Theory and Computation*, **2015**, 11, 45-54	6.4	21
83	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
82	A perspective on the electronic structure calculations for properties of battery electrode materials. *International Journal of Quantum Chemistry*, **2015**, 115, 1141-1146	2.1	4
81	Systematic Investigation of the Effect of Polymerization Routes on the Gas-Sorption Properties of Nanoporous Azobenzene Polymers. *Chemistry - A European Journal*, **2015**, 21, 15320-7	4.8	34
80	Skeletal octahedral nanoframe with Cartesian coordinates via geometrically precise nanoscale phase segregation in a Pt@Ni core-shell nanocrystal. *ACS Nano*, **2015**, 9, 2856-67	16.7	153
79	Modulating the magnetic behavior of Fe(II)-MOF-74 by the high electron affinity of the guest molecule. *Physical Chemistry Chemical Physics*, **2015**, 17, 16977-82	3.6	18
78	The High Performance of Crystal Water Containing Manganese Birnessite Cathodes for Magnesium Batteries. *Nano Letters*, **2015**, 15, 4071-9	11.5	339

77	Exploring the possibilities of two-dimensional transition metal carbides as anode materials for sodium batteries. *Physical Chemistry Chemical Physics*, **2015**, 17, 5000-5	3.6	118
76	Improved reversibility in lithium-oxygen battery: understanding elementary reactions and surface charge engineering of metal alloy catalyst. *Scientific Reports*, **2014**, 4, 4225	4.9	126
75	Carbon nanofluidics of rapid water transport for energy applications. *Chemical Society Reviews*, **2014**, 43, 565-76	58.5	146
74	Can Metal-Organic Framework Separate 1-Butene from Butene Isomers?. *Journal of Physical Chemistry Letters*, **2014**, 5, 440-6	6.4	23
73	Hydrogen-bond-assisted controlled C-H functionalization via adaptive recognition of a purine directing group. *Journal of the American Chemical Society*, **2014**, 136, 1132-40	16.4	132
72	Directing the structural features of N(2)-phobic nanoporous covalent organic polymers for CO(2) capture and separation. *Chemistry - A European Journal*, **2014**, 20, 772-80	4.8	113
71	Role of intermediate phase for stable cycling of Na7V4(P2O7)4PO4 in sodium ion battery. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 599-604	11.5	120
70	Ordered supramolecular gels based on graphene oxide and tetracationic cyclophanes. *Advanced Materials*, **2014**, 26, 2725-9, 2617	24	24
69	Assessments of semilocal density functionals and corrections for carbon dioxide adsorption on metal-organic frameworks. *ChemPhysChem*, **2014**, 15, 3157-65	3.2	11
68	The binding nature of light hydrocarbons on Fe/MOF-74 for gas separation. *Physical Chemistry Chemical Physics*, **2013**, 15, 19644-50	3.6	39
67	Flow-induced voltage generation over monolayer graphene in the presence of herringbone grooves. *Nanoscale Research Letters*, **2013**, 8, 487	5	19
66	Origin of Selective Guest-Induced Magnetism Transition in Fe/MOF-74. *Journal of Physical Chemistry Letters*, **2013**, 4, 2530-2534	6.4	43
65	Unprecedented high-temperature CO2 selectivity in N2-phobic nanoporous covalent organic polymers. *Nature Communications*, **2013**, 4, 1357	17.4	395
64	Molecular dynamics simulations for thermal transport behavior of InAs nanotubes: A role of symmetry. *Computational Materials Science*, **2013**, 70, 8-12	3.2	2
63	Anomalous manganese activation of a pyrophosphate cathode in sodium ion batteries: a combined experimental and theoretical study. *Journal of the American Chemical Society*, **2013**, 135, 2787-92	16.4	131
62	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
61	Highly Stable Nanoporous Sulfur-Bridged Covalent Organic Polymers for Carbon Dioxide Removal. *Advanced Functional Materials*, **2013**, 23, 2270-2276	15.6	126
60	Na2FeP2O7 as a Promising Iron-Based Pyrophosphate Cathode for Sodium Rechargeable Batteries: A Combined Experimental and Theoretical Study. *Advanced Functional Materials*, **2013**, 23, 1147-1155	15.6	250

59	Strengthening effect of single-atomic-layer graphene in metal-graphene nanolayered composites. *Nature Communications*, **2013**, 4, 2114	17.4	418
58	On the structure of Si(100) surface: importance of higher order correlations for buckled dimer. *Journal of Chemical Physics*, **2013**, 138, 204709	3.9	5
57	Between scylla and charybdis: hydrophobic graphene-guided water diffusion on hydrophilic substrates. *Scientific Reports*, **2013**, 3, 2309	4.9	53
56	Flow-induced voltage generation in non-ionic liquids over monolayer graphene. *Applied Physics Letters*, **2013**, 102, 063116	3.4	42
55	Reply to Comment on "On the optimal symmetric purification scheme of the one-particle density matrix" *Chemical Physics Letters*, **2012**, 527, 86-88	2.5	
54	Predictions of the sulfur and carbon kinetic isotope effects in the OH + OCS reaction. *Chemical Physics Letters*, **2012**, 531, 64-69	2.5	16
53	Ab Initio Study of the Sodium Intercalation and Intermediate Phases in Na0.44MnO2 for Sodium-Ion Battery. *Chemistry of Materials*, **2012**, 24, 1205-1211	9.6	195
52	Electrochemical and Thermal Properties of NASICON Structured Na3V2(PO4)3as a Sodium Rechargeable Battery Cathode: A Combined Experimental and Theoretical Study. *Journal of the Electrochemical Society*, **2012**, 159, A1393-A1397	3.9	275
51	Correction and Addition to "Tuning Metal-Organic Frameworks with Open-Metal Sites and Its Origin for Enhancing CO2 Affinity by Metal Substitution". *Journal of Physical Chemistry Letters*, **2012**, 3, 1582	6.4	4
50	Stability of Positively Charged Solutes in Water: A Transition from Hydrophobic to Hydrophilic. *Journal of Physical Chemistry Letters*, **2012**, 3, 294-8	6.4	8
49	Combinatorial screening of highly active Pd binary catalysts for electrochemical oxygen reduction. *ACS Combinatorial Science*, **2012**, 14, 10-6	3.9	33
48	Rollover cyclometalation pathway in rhodium catalysis: dramatic NHC effects in the C-H bond functionalization. *Journal of the American Chemical Society*, **2012**, 134, 17778-88	16.4	139
47	Accurate Ab Initio-Based Force Field for Predictive CO2 Uptake Simulations in MOFs and ZIFs: Development and Applications for MTV-MOFs. *Journal of Physical Chemistry C*, **2012**, 116, 20254-20261	3.8	36
46	On the absolute thermodynamics of water from computer simulations: a comparison of first-principles molecular dynamics, reactive and empirical force fields. *Journal of Chemical Physics*, **2012**, 137, 244507	3.9	51
45	High capacity carbon dioxide adsorption by inexpensive covalent organic polymers. *Journal of Materials Chemistry*, **2012**, 22, 8431		162
44	Site-specific transition metal occupation in multicomponent pyrophosphate for improved electrochemical and thermal properties in lithium battery cathodes: a combined experimental and theoretical study. *Journal of the American Chemical Society*, **2012**, 134, 11740-8	16.4	29
43	Tuning Metal-Organic Frameworks with Open-Metal Sites and Its Origin for Enhancing CO2 Affinity by Metal Substitution. *Journal of Physical Chemistry Letters*, **2012**, 3, 826-9	6.4	103
42	Local intermolecular interactions for selective CO2 capture by zeolitic imidazole frameworks: energy decomposition analysis. *Journal of Nanoparticle Research*, **2012**, 14, 1	2.3	8

41	Size effect of RhPt bimetallic nanoparticles in catalytic activity of CO oxidation: Role of surface segregation. *Catalysis Today*, **2012**, 181, 133-137	5.3	47
40	Local intermolecular interactions for selective CO2 capture by zeolitic imidazole frameworks: energy decomposition analysis **2012**, 277-288		
39	On the mechanism of enhanced oxygen reduction reaction in nitrogen-doped graphene nanoribbons. *Physical Chemistry Chemical Physics*, **2011**, 13, 17505-10	3.6	588
38	Microscopic structure and dynamics of air/water interface by computer simulations--comparison with sum-frequency generation experiments. *Physical Chemistry Chemical Physics*, **2011**, 13, 5388-93	3.6	14
37	Amidoximes: promising candidates for CO2 capture. *Energy and Environmental Science*, **2011**, 4, 4528	35.4	70
36	Accelerated Purification Using Generalized Nonpurifying Intermediate Functions for Large-Scale Self-Consistent Field Calculations. *Journal of Chemical Theory and Computation*, **2011**, 7, 3853-8	6.4	6
35	Intramolecular aromatic carbenoid insertion of biaryldiazoacetates for the regioselective synthesis of fluorenes. *Chemistry - an Asian Journal*, **2011**, 6, 2040-7	4.5	26
34	On the optimal symmetric purification scheme of the one-particle density matrix. *Chemical Physics Letters*, **2011**, 511, 159-160	2.5	4
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