Yousung Jung

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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	Advances in methods and algorithms in a modern quantum chemistry program package. *Physical Chemistry Chemical Physics*, **2006**, 8, 3172-91	3.6	2371
201	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
200	On the mechanism of enhanced oxygen reduction reaction in nitrogen-doped graphene nanoribbons. *Physical Chemistry Chemical Physics*, **2011**, 13, 17505-10	3.6	588
199	On the nature of organic catalysis "on water". *Journal of the American Chemical Society*, **2007**, 129, 5492-502	14.4	506
198	Nitrogen Fixation by Ru Single-Atom Electrocatalytic Reduction. *CheM*, **2019**, 5, 204-214	16.2	501
197	Scaled opposite-spin second order M□ller-Plesset correlation energy: an economical electronic structure method. *Journal of Chemical Physics*, **2004**, 121, 9793-802	3.9	440
196	Strengthening effect of single-atomic-layer graphene in metal-graphene nanolayered composites. *Nature Communications*, **2013**, 4, 2114	17.4	418
195	Unprecedented high-temperature CO2 selectivity in N2-phobic nanoporous covalent organic polymers. *Nature Communications*, **2013**, 4, 1357	17.4	395
194	The High Performance of Crystal Water Containing Manganese Birnessite Cathodes for Magnesium Batteries. *Nano Letters*, **2015**, 15, 4071-9	11.5	339
193	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
192	Active Sites of Au and Ag Nanoparticle Catalysts for CO2Electroreduction to CO. *ACS Catalysis*, **2015**, 5, 5089-5096	13.1	326
191	Single-atom catalysts for CO electroreduction with significant activity and selectivity improvements. *Chemical Science*, **2017**, 8, 1090-1096	9.4	319
190	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
189	Entropy and the driving force for the filling of carbon nanotubes with water. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 11794-8	11.5	251
188	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
187	Intermolecular pi-to-pi bonding between stacked aromatic dyads. Experimental and theoretical binding energies and near-IR optical transitions for phenalenyl radical/radical versus radical/cation dimerizations. *Journal of the American Chemical Society*, **2004**, 126, 13850-8	16.4	249
186	Two-Dimensional Transition Metal Dichalcogenide Monolayers as Promising Sodium Ion Battery Anodes. *Journal of Physical Chemistry C*, **2015**, 119, 26374-26380	3.8	210

185	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
184	Auxiliary basis expansions for large-scale electronic structure calculations. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 6692-7	11.5	171
183	Balancing activity, stability and conductivity of nanoporous core-shell iridium/iridium oxide oxygen evolution catalysts. *Nature Communications*, **2017**, 8, 1449	17.4	168
182	High capacity carbon dioxide adsorption by inexpensive covalent organic polymers. *Journal of Materials Chemistry*, **2012**, 22, 8431		162
181	Hydrated Intercalation for High-Performance Aqueous Zinc Ion Batteries. *Advanced Energy Materials*, **2019**, 9, 1900083	21.8	158
180	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
179	Carbon nanofluidics of rapid water transport for energy applications. *Chemical Society Reviews*, **2014**, 43, 565-76	58.5	146
178	Critical Role of Crystal Water for a Layered Cathode Material in Sodium Ion Batteries. *Chemistry of Materials*, **2015**, 27, 3721-3725	9.6	142
177	Heterogeneous Catalysis for Lithium–Sulfur Batteries: Enhanced Rate Performance by Promoting Polysulfide Fragmentations. *ACS Energy Letters*, **2017**, 2, 327-333	20.1	141
176	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
175	Selective Heterogeneous CO2 Electroreduction to Methanol. *ACS Catalysis*, **2015**, 5, 965-971	13.1	137
174	Selective nitrogen capture by porous hybrid materials containing accessible transition metal ion sites. *Nature Materials*, **2017**, 16, 526-531	27	135
173	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
172	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
171	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
170	Activated TiO2 with tuned vacancy for efficient electrochemical nitrogen reduction. *Applied Catalysis B: Environmental*, **2019**, 257, 117896	21.8	130
169	Porous cationic polymers: the impact of counteranions and charges on CO2 capture and conversion. *Chemical Communications*, **2016**, 52, 934-7	5.8	127
168	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

167	Highly Stable Nanoporous Sulfur-Bridged Covalent Organic Polymers for Carbon Dioxide Removal. *Advanced Functional Materials*, **2013**, 23, 2270-2276	15.6	126
166	A fast doubly hybrid density functional method close to chemical accuracy using a local opposite spin ansatz. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 19896-900	11.5	124
165	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
164	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
163	Carbon-supported Ni nanoparticles for efficient CO electroreduction. *Chemical Science*, **2018**, 9, 8775-8780	9.4	116
162	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
161	Machine learning for renewable energy materials. *Journal of Materials Chemistry A*, **2019**, 7, 17096-17117	13	114
160	New Insights into the Structure of the Vapor/Water Interface from Large-Scale First-Principles Simulations. *Journal of Physical Chemistry Letters*, **2011**, 2, 105-13	6.4	114
159	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
158	On the mechanism of electrochemical ammonia synthesis on the Ru catalyst. *Physical Chemistry Chemical Physics*, **2016**, 18, 9161-6	3.6	111
157	Activation of Ni Particles into Single Ni□N Atoms for Efficient Electrochemical Reduction of CO2. *Advanced Energy Materials*, **2020**, 10, 1903068	21.8	111
156	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
155	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
154	Inverse Design of Solid-State Materials via a Continuous Representation. *Matter*, **2019**, 1, 1370-1384	12.7	99
153	How diradicaloid is a stable diradical?. *ChemPhysChem*, **2003**, 4, 522-5	3.2	95
152	Oxygen vacancy enables electrochemical N2 fixation over WO3 with tailored structure. *Nano Energy*, **2019**, 62, 869-875	17.1	94
151	Ab initio quantum chemistry calculations on the electronic structure of heavier alkyne congeners: diradical character and reactivity. *Journal of the American Chemical Society*, **2006**, 128, 7185-92	16.4	86
150	What is the nature of the long bond in the TCNE2□□dimer?. *Physical Chemistry Chemical Physics*, **2004**, 6, 2008-2011	3.6	83

149	A Resolution-Of-The-Identity Implementation of the Local Triatomics-In-Molecules Model for Second-Order MÖller-Plesset Perturbation Theory with Application to Alanine Tetrapeptide Conformational Energies. *Journal of Chemical Theory and Computation*, **2005**, 1, 862-76	6.4	82
148	Scaled opposite spin second order MÖller-Plesset theory with improved physical description of long-range dispersion interactions. *Journal of Physical Chemistry A*, **2005**, 109, 7598-605	2.8	78
147	Aromaticity of four-membered-ring 6pi-electron systems: N2S2 and Li2C4H4. *Journal of the American Chemical Society*, **2004**, 126, 3132-8	16.4	75
146	Doping palladium with tellurium for the highly selective electrocatalytic reduction of aqueous CO to CO. *Chemical Science*, **2018**, 9, 483-487	9.4	73
145	High-yield production of few-layer boron nanosheets for efficient electrocatalytic N reduction. *Chemical Communications*, **2019**, 55, 4246-4249	5.8	71
144	Amidoximes: promising candidates for CO2 capture. *Energy and Environmental Science*, **2011**, 4, 4528	35.4	70
143	Electrochemical ammonia synthesis: Mechanistic understanding and catalyst design. *CheM*, **2021**, 7, 1708-1754	16.2	70
142	The Role of Adsorbed CN and Cl on an Au Electrode for Electrochemical CO2 Reduction. *ACS Catalysis*, **2018**, 8, 1178-1185	13.1	67
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139	A fast correlated electronic structure method for computing interaction energies of large van der Waals complexes applied to the fullerene-porphyrin dimer. *Physical Chemistry Chemical Physics*, **2006**, 8, 2831-40	3.6	61
138	Boosting hot electron flux and catalytic activity at metal-oxide interfaces of PtCo bimetallic nanoparticles. *Nature Communications*, **2018**, 9, 2235	17.4	56
137	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
136	Highly stable two-dimensional bismuth metal-organic frameworks for efficient electrochemical reduction of CO2. *Applied Catalysis B: Environmental*, **2020**, 277, 119241	21.8	53
135	Adsorbate-driven reactive interfacial Pt-NiO nanostructure formation on the PtNi(111) alloy surface. *Science Advances*, **2018**, 4, eaat3151	14.3	53
134	Between scylla and charybdis: hydrophobic graphene-guided water diffusion on hydrophilic substrates. *Scientific Reports*, **2013**, 3, 2309	4.9	53
133	Fast evaluation of scaled opposite spin second-order MÖller-Plesset correlation energies using auxiliary basis expansions and exploiting sparsity. *Journal of Computational Chemistry*, **2007**, 28, 1953-64	3.5	53
132	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

131	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
130	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
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127	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
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125	Phenol-benzene complexation dynamics: quantum chemistry calculation, molecular dynamics simulations, and two dimensional IR spectroscopy. *Journal of Chemical Physics*, **2006**, 125, 244508	3.9	47
124	Cycloaddition of benzene on Si(100) and its surface conversions. *Journal of the American Chemical Society*, **2005**, 127, 3131-9	16.4	47
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122	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
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119	Flow-induced voltage generation in non-ionic liquids over monolayer graphene. *Applied Physics Letters*, **2013**, 102, 063116	3.4	42
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116	The binding nature of light hydrocarbons on Fe/MOF-74 for gas separation. *Physical Chemistry Chemical Physics*, **2013**, 15, 19644-50	3.6	39
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114	Adsorption of Water on the Si(100) Surface: An Ab Initio and QM/MM Cluster Study. *Journal of Physical Chemistry B*, **2001**, 105, 4039-4044	3.4	38

113	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
112	Generative Adversarial Networks for Crystal Structure Prediction. *ACS Central Science*, **2020**, 6, 1412-1420	6.8	35
111	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
110	Stabilization of Cu+ by tuning a CuO□eO2 interface for selective electrochemical CO2 reduction to ethylene. *Green Chemistry*, **2020**, 22, 6540-6546	10	34
109	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
108	Combinatorial screening of highly active Pd binary catalysts for electrochemical oxygen reduction. *ACS Combinatorial Science*, **2012**, 14, 10-6	3.9	33
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106	Efficient visible-light driven N fixation over two-dimensional Sb/TiO composites. *Chemical Communications*, **2019**, 55, 7171-7174	5.8	31
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104	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
103	Diamine-Functionalization of a Metal-Organic Framework Adsorbent for Superb Carbon Dioxide Adsorption and Desorption Properties. *ChemSusChem*, **2018**, 11, 1694-1707	8.3	30
102	Practical Deep-Learning Representation for Fast Heterogeneous Catalyst Screening. *Journal of Physical Chemistry Letters*, **2020**, 11, 3185-3191	6.4	29
101	Understanding the Effects of Au Morphology on CO2 Electrocatalysis. *Journal of Physical Chemistry C*, **2018**, 122, 4274-4280	3.8	29
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97	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
96	Ordered supramolecular gels based on graphene oxide and tetracationic cyclophanes. *Advanced Materials*, **2014**, 26, 2725-9, 2617	24	24

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94	Origin of unusual spinel-to-layered phase transformation by crystal water. *Chemical Science*, **2018**, 9, 433-438	9.4	23
93	Can Metal-Organic Framework Separate 1-Butene from Butene Isomers?. *Journal of Physical Chemistry Letters*, **2014**, 5, 440-6	6.4	23
92	Multilayer Two-Dimensional Water Structure Confined in MoS2. *Journal of Physical Chemistry C*, **2017**, 121, 16021-16028	3.8	23
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90	Understanding potential-dependent competition between electrocatalytic dinitrogen and proton reduction reactions. *Nature Communications*, **2021**, 12, 4353	17.4	22
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88	Importance of Ligand Effects Breaking the Scaling Relation for Core□Shell Oxygen Reduction Catalysts. *ChemCatChem*, **2017**, 9, 3173-3179	5.2	21
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86	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
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83	Effects of boron oxidation state on electrocatalytic activity of carbons synthesized from CO2. *Journal of Materials Chemistry A*, **2015**, 3, 5843-5849	13	20
82	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
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80	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
79	Flow-induced voltage generation over monolayer graphene in the presence of herringbone grooves. *Nanoscale Research Letters*, **2013**, 8, 487	5	19
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76	Probing surface oxide formations on SiO2-supported platinum nanocatalysts under CO oxidation. *RSC Advances*, **2017**, 7, 45003-45009	3.7	18
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73	An ab initio study of the structure of two-, three- and five-dimersilicon clusters: An approach to the Si(100) surface. *Theoretical Chemistry Accounts*, **2003**, 109, 268-273	1.9	18
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45	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
44	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
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