Yoong-Kee Choe

List of Publications by Year
in descending order

60 papers	2,356 citations	218592 26 h-index	206029 48 g-index
61 all docs	61 docs citations	61 times ranked	2671 citing authors

#	Article	IF	Citations
1	Systematic Alkaline Stability Study of Polymer Backbones for Anion Exchange Membrane Applications. Macromolecules, 2016, 49, 3361-3372.	2.2	287
2	An operationally flexible fuel cell based on quaternary ammonium-biphosphate ion pairs. Nature Energy, 2016, 1, .	19.8	206
3	Intruder state avoidance multireference MÃ¸ller-Plesset perturbation theory. Journal of Computational Chemistry, 2002, 23, 957-965.	1.5	186
4	Theoretical Study of the Q and B Bands of Free-Base, Magnesium, and Zinc Porphyrins, and Their Derivatives. Journal of Physical Chemistry A, 1999, 103, 1894-1904.	1.1	157
5	Alkaline Stability of Benzyl Trimethyl Ammonium Functionalized Polyaromatics: A Computational and Experimental Study. Chemistry of Materials, 2014, 26, 5675-5682.	3.2	152
6	Nature of proton dynamics in a polymer electrolyte membrane, nafion: a first-principles molecular dynamics study. Physical Chemistry Chemical Physics, 2009, 11, 3892.	1.3	93
7	Resonance Stabilized Perfluorinated Ionomers for Alkaline Membrane Fuel Cells. Macromolecules, 2013, 46, 7826-7833.	2.2	90
8	The energetics of phosphoric acid interactions reveals a new acid loss mechanism. Journal of Materials Chemistry A, 2019, 7, 9867-9876.	5.2	83
9	Synthesis, Structure, and Reactivity of Hydridoiridium Complexes Bearing a Pincerâ€Type PSiP Ligand. Chemistry - an Asian Journal, 2011, 6, 2512-2521.	1.7	80
10	Theoretical study of the electronic ground state of iron(II) porphine. II. Journal of Chemical Physics, 1999, 111, 3837-3845.	1.2	76
11	Identifying and removing intruder states in multireference Mo/llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 2001, 114, 3913-3918.	1.2	61
12	Multireference MÃ¸llerâ€“Plesset method with a complete active space configuration interaction reference function. Journal of Chemical Physics, 2001, 115, 621-629.	1.2	59
13	First-principles molecular dynamics study on aqueous sulfuric acid solutions. Journal of Chemical Physics, 2007, 126, 154510.	1.2	55
14	Nature of Water Transport and Electro-Osmosis in Nafion: Insights from First-Principles Molecular Dynamics Simulations under an Electric Field. Journal of Physical Chemistry B, 2008, 112, 11586-11594.	1.2	51
15	Multinuclear palladium compounds containing palladium centers ligated by five silicon atoms. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 7758-7763.	3.3	47
16	Isolation of aSe-Nitrososelenol:Â A New Class of Reactive Nitrogen Species Relevant to ProteinSe-Nitrosation. Journal of the American Chemical Society, 2004, 126, 13238-13239.	6.6	46
17	Theoretical study of the electronic ground state of iron(II) porphine. Chemical Physics Letters, 1998, 295, 380-388.	1.2	39
18	An Ab Initio Modeling Study on a Modeled Hydrated Polymer Electrolyte Membrane, Sulfonated Polyethersulfone (SPES). Journal of Physical Chemistry B, 2010, 114, 2411-2421.	1.2	38

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19	Theoretical study of the electronic spectra of oxidized and reduced states of lumiflavin and its derivative. Journal of Computational Chemistry, 2007, 28, 727-739.	1.5	36
20	Effect of Substituents on the Thermal Decomposition of Diazirines:Â Experimental and Computational Studies. Journal of Organic Chemistry, 2003, 68, 7471-7478.	1.7	32
21	A unique Biâ€“Bi bond forming reaction using organobismuth oxides and phosphorus compounds bearing a P(î€Ō)H group. Chemical Communications, 2009, , 6168.	2.2	32
22	Theoretical studies on the degradation of hydrocarbon copolymer ionomers used in fuel cells. Journal of Membrane Science, 2015, 487, 229-239.	4.1	32
23	Olefin hydrosilylation catalyzed by cationic nickel(<scp>ii</scp>) allyl complexes: a non-innocent allyl ligand-assisted mechanism. Chemical Communications, 2016, 52, 6723-6726.	2.2	32
24	A comparison of the photochemical reactivity of N@C60 and C60: photolysis with disiliraneElectronic supplementary information (ESI) available: experimental results. See http://www.rsc.org/suppdata/cc/b3/b309470g/. Chemical Communications, 2003, , 2940.	2.2	30
25	Effect of Organic Cations on Hydrogen Oxidation Reaction of Carbon Supported Platinum. Journal of the Electrochemical Society, 2016, 163, F1503-F1509.	1.3	29
26	A CASCI-MRMP method based on Kohnâ€”Sham orbitals. Molecular Physics, 2002, 100, 729-745.	0.8	27
27	Turning Harmful Deposition of Metal Impurities into Activation of Nitrogen-Doped Carbon Catalyst toward Durable Electrochemical CO₂ Reduction. ACS Energy Letters, 2019, 4, 2343-2350.	8.8	23
28	Theoretical identification ofC20carbon clusters:â€ƒPrevalence of the monocyclic isomer and existence of the smallest fullerene and bowl isomer. Physical Review B, 2003, 67, .	1.1	22
29	[Pd(4-R₃Si-IPr)(allyl)Cl], a Family of Silyl-Substituted Pdâ€“NHC Complexes: Catalytic Systems for the Buchwaldâ€“Hartwig Amination. Organometallics, 2019, 38, 375-384.	1.1	22
30	Suppressing vanadium crossover using sulfonated aromatic ion exchange membranes for high performance flow batteries. Materials Advances, 2020, 1, 2206-2218.	2.6	22
31	Ab initio studies on the proton dissociation and infrared spectra of sulfonated poly(ether ether) Tj ETQq1 1 0.784314 rgBT /Overlock	1.3	20
32	An adaptive finite-element method for large-scale ab initio molecular dynamics simulations. Physical Chemistry Chemical Physics, 2015, 17, 31444-31452.	1.3	18
33	Calculation of packing structure of methanol solid using ab initio lattice energy at the MP2 level. Chemical Physics Letters, 2003, 369, 597-604.	1.2	15
34	Effect of the axial cysteine ligand on the electronic structure and reactivity of high-valent iron(IV) oxo-porphyrins (Compound I): A theoretical study. Journal of Computational Chemistry, 2005, 26, 1600-1611.	1.5	15
35	DFT Studies of Perfluorosulfonic Acid Ionomer Degradation in Fuel Cells. Journal of Physical Chemistry C, 2018, 122, 20135-20143.	1.5	15
36	Alkoxysilane production from silica and dimethylcarbonate catalyzed by alkali bases: A quantum chemical investigation of the reaction mechanism. Inorganica Chimica Acta, 2018, 482, 70-76.	1.2	13

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37	Fundamental roles of ZnO and ZrO₂in the conversion of ethanol to 1,3-butadiene over ZnOâ€“ZrO₂/SiO₂. Catalysis Science and Technology, 2020, 10, 7531-7541.	2.1	13
38	Mechanistic investigation on ethanolâ€toâ€butadiene conversion reaction over metal oxide clusters. International Journal of Quantum Chemistry, 2021, 121, e26494.	1.0	13
39	Nâ€Aryl and Nâ€Alkyl Carbamates from 1 Atmosphere of CO₂. Chemistry - A European Journal, 2021, 27, 18066-18073.	1.7	12
40	Iterative diagonalization of symmetric matrices in mixed precision and its application to electronic structure calculations. Computer Physics Communications, 2012, 183, 980-985.	3.0	11
41	Tris(pentafluorophenyl)boraneâ€Catalyzed Reactions of Siloxanes: A Combined Experimental and Computational Study. European Journal of Organic Chemistry, 2017, 2017, 4922-4927.	1.2	9
42	Vibrational analysis of aqueous sulfuric acid: A computational study. International Journal of Quantum Chemistry, 2009, 109, 1984-1990.	1.0	8
43	Theoretical Studies of Pendant Effects on the Properties of Sulfonated Hydrocarbon Polymer Electrolyte Membranes. Journal of Physical Chemistry C, 2015, 119, 11362-11369.	1.5	7
44	On the performance of diagrammatic complete active space perturbation theory. Journal of Chemical Physics, 2000, 113, 7773-7778.	1.2	6
45	First-Principles Molecular Dynamics Study of a Hydrocarbon Copolymer for Use in Polymer Electrolyte Membrane Fuel Cells. Journal of Physical Chemistry C, 2016, 120, 13398-13405.	1.5	6
46	Theoretical Study of the Mechanism for the Reaction of Trimethylaluminum with Ozone. ACS Omega, 2021, 6, 26282-26292.	1.6	5
47	[Pd(4-RSi-IPr)(allyl)Cl]/KCO/EtOH: A highly effective catalytic system for the Suzuki-Miyaura cross-coupling reaction. Journal of Organometallic Chemistry, 2021, 954-955, 122096.	0.8	5
48	Structure dependency of the reactivity of aromatic hydrocarbons involving the formation of oxygenated polycyclic aromatic hydrocarbons (OPAHs). Chemical Physics Letters, 2020, 754, 137652.	1.2	4
49	Electrical property of a sulfuric acidâ€“water mixture from the first-principles molecular dynamics simulation. Computer Physics Communications, 2007, 177, 38-39.	3.0	3
50	Understanding properties of copoly(arylene ether nitrile)s high-performance polymer electrolyte membranes for fuel cells from molecular dynamics simulations. Theoretical Chemistry Accounts, 2011, 130, 555-561.	0.5	3
51	Synthesis, structure and properties of trivalent and pentavalent tricarbabismatranes. Chemical Communications, 2022, 58, 6614-6617.	2.2	3
52	Proton Dynamics in a Polymer Electrolyte Membrane, Sulfonated Polyether Sulfone (SPES): A Computational Study. ECS Transactions, 2009, 25, 1075-1083.	0.3	2
53	Theoretical study of the side reactions of the catalytic conversion of ethanol to butadiene on metal oxide catalysts. Catalysis Communications, 2021, 149, 106239.	1.6	2
54	First-principles molecular dynamics simulation study on Ti4+ ion in aqueous sulfuric acid. AIP Advances, 2021, 11, 035224.	0.6	2

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55	Mechanistic Details on the Conversion of Siâ€“O to Siâ€“C Bonds Using Metal Hydrides: A Density Functional Theory Study. European Journal of Inorganic Chemistry, 2019, 2019, 1335-1342.	1.0	1
56	Molecular Design Aspect of Anion Exchange Polymer Electrolytes. ECS Transactions, 2013, 58, 417-423.	0.3	0
57	Chemical degradation mechanisms of membranes for alkaline membrane fuel cells. AIP Conference Proceedings, 2015, , .	0.3	0
58	A DFT Study on the Dissociation Property of Sulfonic Acids with Different Neighboring Pendants in Polymer Electrolyte Membranes. , 2015, , .		0
59	Computational modeling study on polymer electrolyte membranes for fuel cell applications. AIP Conference Proceedings, 2016, , .	0.3	0
60	First-principles molecular dynamics simulation study on electrolytes for use in redox flow battery. AIP Conference Proceedings, 2017, , .	0.3	0