

# Ki Chul Kim

## List of Publications by Year in descending order

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79  
papers

2,883  
citations

201575

27  
h-index

175177

52  
g-index

81  
all docs

81  
docs citations

81  
times ranked

3874  
citing authors

#	ARTICLE	IF	CITATIONS
1	High Propene/Propane Selectivity in Isostructural Metal-Organic Frameworks with High Densities of Open Metal Sites. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 1857-1860.	7.2	392
2	An Extended Charge Equilibration Method. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2506-2511.	2.1	253
3	Self-polymerized dopamine as an organic cathode for Li- and Na-ion batteries. <i>Energy and Environmental Science</i> , 2017, 10, 205-215.	15.6	253
4	First-Principles Density Functional Theory Modeling of Li Binding: Thermodynamics and Redox Properties of Quinone Derivatives for Lithium-Ion Batteries. <i>Journal of the American Chemical Society</i> , 2016, 138, 2374-2382.	6.6	194
5	Assessing nanoparticle size effects on metal hydride thermodynamics using the Wulff construction. <i>Nanotechnology</i> , 2009, 20, 204001.	1.3	127
6	Applicability of using CO <sub>2</sub> adsorption isotherms to determine BET surface areas of microporous materials. <i>Microporous and Mesoporous Materials</i> , 2016, 224, 294-301.	2.2	112
7	Application of DFT-based machine learning for developing molecular electrode materials in Li-ion batteries. <i>RSC Advances</i> , 2018, 8, 39414-39420.	1.7	96
8	High-Density Lithium-Ion Energy Storage Utilizing the Surface Redox Reactions in Folded Graphene Films. <i>Chemistry of Materials</i> , 2015, 27, 3291-3298.	3.2	78
9	Modeling Water and Ammonia Adsorption in Hydrophobic Metal-Organic Frameworks: Single Components and Mixtures. <i>Journal of Physical Chemistry C</i> , 2014, 118, 1102-1110.	1.5	57
10	Crystal Structures and Thermodynamic Investigations of LiK(BH <sub>4</sub> ) <sub>2</sub> , KBH <sub>4</sub> , and NaBH <sub>4</sub> from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2010, 114, 678-686.	1.5	56
11	A review on design strategies for metal hydrides with enhanced reaction thermodynamics for hydrogen storage applications. <i>International Journal of Energy Research</i> , 2018, 42, 1455-1468.	2.2	56
12	AZn <sub>2</sub> (BH <sub>4</sub> ) <sub>5</sub> (A = Li, Na) and NaZn(BH <sub>4</sub> ) <sub>3</sub> : Structural Studies. <i>Journal of Physical Chemistry C</i> , 2010, 114, 19127-19133.	1.5	53
13	Selective dynamic separation of Xe and Kr in Co-MOF-74 through strong binding strength between Xe atom and unsaturated Co <sup>2+</sup> site. <i>Microporous and Mesoporous Materials</i> , 2016, 236, 284-291.	2.2	52
14	Computational Screening of Functional Groups for Ammonia Capture in Metal-Organic Frameworks. <i>Langmuir</i> , 2013, 29, 1446-1456.	1.6	49
15	Design Strategies for Promising Organic Positive Electrodes in Lithium-Ion Batteries: Quinones and Carbon Materials. <i>Industrial &amp; Engineering Chemistry Research</i> , 2017, 56, 12009-12023.	1.8	49
16	Molecular Dynamics Simulations of Aldol Condensation Catalyzed by Alkylamine-Functionalized Crystalline Silica Surfaces. <i>Journal of the American Chemical Society</i> , 2016, 138, 7664-7672.	6.6	44
17	Systematic Molecular Design of Ketone Derivatives of Aromatic Molecules for Lithium-Ion Batteries: First-Principles DFT Modeling. <i>ChemSusChem</i> , 2017, 10, 1584-1591.	3.6	44
18	Thermodynamic and redox properties of graphene oxides for lithium-ion battery applications: a first principles density functional theory modeling approach. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20600-20606.	1.3	39

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19	Electrochemical Properties of Boron-Doped Fullerene Derivatives for Lithium-Ion Battery Applications. <i>ChemPhysChem</i> , 2018, 19, 753-758.	1.0	37
20	Electrochemical and electronic properties of nitrogen doped fullerene and its derivatives for lithium-ion battery applications. <i>Journal of Energy Chemistry</i> , 2018, 27, 528-534.	7.1	36
21	Design strategies for metal-organic frameworks selectively capturing harmful gases. <i>Journal of Organometallic Chemistry</i> , 2018, 854, 94-105.	0.8	34
22	Conjugacy of organic cathode materials for high-potential lithium-ion batteries: Carbonitriles versus quinones. <i>Energy Storage Materials</i> , 2020, 24, 237-246.	9.5	33
23	Unveiled correlations between electron affinity and solvation in redox potential of quinone-based sodium-ion batteries. <i>Energy Storage Materials</i> , 2019, 19, 242-250.	9.5	32
24	Large-scale screening of metal hydrides for hydrogen storage from first-principles calculations based on equilibrium reaction thermodynamics. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 7218.	1.3	30
25	New fundamental experimental studies on $\text{Li-Mg}(\text{BH}_4)_2$ and other borohydrides. <i>Journal of Alloys and Compounds</i> , 2011, 509, S688-S690.	2.8	29
26	Influence of a UV-ozone treatment on amorphous $\text{SnO}_2$ electron selective layers for highly efficient planar $\text{MAPbI}_3$ perovskite solar cells. <i>Journal of Materials Science and Technology</i> , 2020, 59, 195-202.	5.6	28
27	Computational Screening of Metal Catecholates for Ammonia Capture in Metal-Organic Frameworks. <i>Industrial &amp; Engineering Chemistry Research</i> , 2015, 54, 3257-3267.	1.8	27
28	Density Functional Theory Machine Learning Approach to Analyze the Bandgap of Elemental Halide Perovskites and Ruddlesden-Popper Phases. <i>ChemPhysChem</i> , 2018, 19, 2559-2565.	1.0	27
29	Observation of Olefin/Paraffin Selectivity in Azo Compound and Its Application into a Metal-Organic Framework. <i>ACS Applied Materials &amp; Interfaces</i> , 2018, 10, 27521-27530.	4.0	26
30	Improvement of Electrical Conductivity in Conjugated Polymers through Cascade Doping with Small-Molecular Dopants. <i>Advanced Materials</i> , 2020, 32, e2005129.	11.1	26
31	Boron-doped coronenes with high redox potential for organic positive electrodes in lithium-ion batteries: a first-principles density functional theory modeling study. <i>Journal of Materials Chemistry A</i> , 2018, 6, 10111-10120.	5.2	22
32	Computational Study of Propylene and Propane Binding in Metal-Organic Frameworks Containing Highly Exposed $\text{Cu}^{+}$ or $\text{Ag}^{+}$ Cations. <i>Journal of Physical Chemistry C</i> , 2014, 118, 9086-9092.	1.5	21
33	Well-dispersed carbon nanotube/polymer composite films and application to electromagnetic interference shielding. <i>Journal of Industrial and Engineering Chemistry</i> , 2019, 80, 190-196.	2.9	21
34	Synergistic passivation of $\text{MAPbI}_3$ perovskite solar cells by compositional engineering using acetamidinium bromide additives. <i>Journal of Energy Chemistry</i> , 2021, 59, 755-762.	7.1	21
35	Predicting impurity gases and phases during hydrogen evolution from complex metal hydrides using free energy minimization enabled by first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 9918.	1.3	20
36	Density Functional Theory Modeling-Assisted Investigation of Thermodynamics and Redox Properties of Boron-Doped Corannulenes for Cathodes in Lithium-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2018, 122, 10675-10681.	1.5	20

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37	Enhanced Lithium Storage of an Organic Cathode via the Bipolar Mechanism. <i>ACS Applied Energy Materials</i> , 2020, 3, 3728-3735.	2.5	18
38	Functionalized Fullerenes in Water: A Closer Look. <i>Environmental Science &amp; Technology</i> , 2015, 49, 2147-2155.	4.6	15
39	Improving the Understanding of the Redox Properties of Fluoranil Derivatives for Cathodes in Sodium-Ion Batteries. <i>ChemSusChem</i> , 2019, 12, 4968-4975.	3.6	15
40	Electrochemical Characteristics of Cyanoquinones as Organic Cathodes for High-Potential Sodium-Ion Batteries. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 11328-11336.	3.2	15
41	Toward coupling of electrochemical redox properties with electrostatic potential surfaces tailored by dopant architectures for pyrenetetrone. <i>Energy Storage Materials</i> , 2021, 35, 610-619.	9.5	15
42	New approach for nanoscale morphology of polymer solar cells. <i>Solar Energy Materials and Solar Cells</i> , 2008, 92, 1188-1191.	3.0	14
43	Examining the robustness of first-principles calculations for metal hydride reaction thermodynamics by detection of metastable reaction pathways. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 21520.	1.3	14
44	Enhanced Selectivity for CO <sub>2</sub> Adsorption on Mesoporous Silica with Alkali Metal Halide Due to Electrostatic Field: A Molecular Simulation Approach. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 31683-31690.	4.0	14
45	Pyrenetetrone Derivatives Tailored by Nitrogen Dopants for High-Potential Cathodes in Lithium-Ion Batteries. <i>IScience</i> , 2019, 21, 206-216.	1.9	14
46	Crucial role of cyanides for high-potential electrochemical reduction reaction. <i>Energy Storage Materials</i> , 2020, 29, 140-148.	9.5	14
47	Ambient-air fabrication of stable mixed cation perovskite planar solar cells with efficiencies exceeding 22% using a synergistic mixed antisolvent with complementary properties. <i>Nano Energy</i> , 2021, 89, 106387.	8.2	14
48	Dopant-dependent thermoelectric performance of indoloindole-selenophene based conjugated polymer. <i>Chemical Engineering Journal</i> , 2022, 431, 133779.	6.6	13
49	Li-Binding Thermodynamics and Redox Properties of BNOPS-Based Organic Compounds for Cathodes in Lithium-Ion Batteries. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 31972-31979.	4.0	11
50	Insights on Redox Properties of Sumanene Derivatives for High-Performance Organic Cathodes. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 8333-8341.	4.0	10
51	Unraveling Three-Stage Discharging Behaviors of Bio-Inspired Organic Cathode Materials. <i>Advanced Functional Materials</i> , 2021, 31, 2105285.	7.8	10
52	Molecular Simulation Study on Factors Affecting Carbon Dioxide Adsorption on Amorphous Silica Surfaces. <i>Journal of Physical Chemistry C</i> , 2020, 124, 12580-12588.	1.5	9
53	Solid-state facilitated transport membrane for CO/N <sub>2</sub> separation based on PHMEP-co-PAA comb-like copolymer: Experimental and molecular simulation study. <i>Journal of Membrane Science</i> , 2021, 620, 118939.	4.1	9
54	Instantaneous Detection of Trichlorinated Carbon via Photo-Induced Electron Transfer toward Chemosensor for Toxic Organochlorides. <i>ACS Sensors</i> , 2018, 3, 1831-1837.	4.0	8

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55	Cu(I)-incorporation strategy for developing styrene selective adsorbents. Chemical Engineering Journal, 2021, 425, 130601.	6.6	8
56	Highly CO-Selective Mixed-Matrix membranes incorporated with Ag Nanoparticle-Impregnated MIL-101 Metal-Organic frameworks. Chemical Engineering Journal, 2022, 435, 134803.	6.6	8
57	Fe-Porphyrin-like Nanostructures for Selective Ammonia Capture under Humid Conditions. Journal of Physical Chemistry C, 2018, 122, 2046-2052.	1.5	7
58	Tailored Design of Electrochemically Degradable Anthraquinone Functionality toward Organic Cathodes. ACS Applied Materials & Interfaces, 2021, 13, 35729-35738.	4.0	7
59	Predictions of Sulfur Resistance in Metal Membranes for H <sub>2</sub> Purification Using First-Principles Calculations. Industrial & Engineering Chemistry Research, 2012, 51, 301-309.	1.8	6
60	Crystal structures and thermodynamic investigations of NaSc(BH <sub>4</sub> ) <sub>4</sub> from first-principles calculations. International Journal of Quantum Chemistry, 2013, 113, 119-124.	1.0	6
61	Unveiled Understanding on Thermodynamic Mechanisms of Atomic Layer Deposition Based on Trimethylaluminum and Water Precursors. Industrial & Engineering Chemistry Research, 2020, 59, 13325-13332.	1.8	6
62	Synthesis, structure and gas separation properties of ethanol-soluble, amphiphilic POM-PBHP comb copolymers. Polymer, 2019, 180, 121700.	1.8	5
63	Electrochemical Energy Storage Capability of Pyrenetetrone Derivatives Tailored by Nitrogen Dopants. Journal of Physical Chemistry C, 2020, 124, 10815-10822.	1.5	5
64	Validation of the reaction thermodynamics associated with NaSc(BH <sub>4</sub> ) <sub>4</sub> from first-principles calculations: Detecting metastable paths and identifying the minimum free energy path. Journal of Chemical Physics, 2012, 137, 084111.	1.2	4
65	Molecular dynamics simulation study on the structural properties of poly (ethylene terephthalate) under uniaxial extension and thermal shrinkage processes. Current Applied Physics, 2018, 18, 19-26.	1.1	4
66	Isomorphous Substitution of Copper in Nickel Phosphate and Their Separation of Propylene Over Propane. Journal of Nanoscience and Nanotechnology, 2016, 16, 9141-9148.	0.9	3
67	Tailoring Impact of Carbonyl Functionalities on Electrochemical Redox Properties of Anthraquinone. Journal of Physical Chemistry C, 2021, 125, 8208-8215.	1.5	3
68	Development of computational design for reliable prediction of dielectric strengths of perfluorocarbon compounds. Scientific Reports, 2022, 12, 7027.	1.6	3
69	Blends of poly(3-alkylthiophene) and [6,6]-phenyl-C <sub>61</sub> -butyric acid methyl ester for organic photovoltaic cell applications: Multi-scale modeling approach. Computational Materials Science, 2017, 126, 299-307.	1.4	2
70	Effects of thermal shrinkage temperatures and comonomers on thermal shrinkage of uniaxially-stretched PET copolymer films: a molecular dynamics simulation approach. New Journal of Chemistry, 2018, 42, 4991-4997.	1.4	2
71	Effective Nitrogen Incorporation for High-Potential Anthracene Cathodes with Conjugated Frameworks. Advanced Theory and Simulations, 2022, 5, .	1.3	2
72	Computational screening of functional groups for capture of toxic industrial chemicals in porous materials. Physical Chemistry Chemical Physics, 2017, 19, 31766-31772.	1.3	1

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73	Physisorption and Chemisorption of SF <sub>6</sub> by Transition Metal-Porphyrin Structure Embedded on Graphene Surface with Different Hapticities. Journal of the Korean Physical Society, 2020, 76, 1001-1004.	0.3	1
74	Unveiled Correlations between Electron Affinity and Solvation in Redox Potential of Quinone-Based Sodium-Ion Batteries. SSRN Electronic Journal, 0, , .	0.4	1
75	Strategic Design for Sumanene-Derived Organic Cathodes with Tailored Redox Activity. Advanced Theory and Simulations, 2022, 5, .	1.3	1
76	Mechanistic Mapping of Ozone-Dosed Al <sub>2</sub> O <sub>3</sub> Atomic Layer Deposition Half-Cycles. Industrial & Engineering Chemistry Research, 2022, 61, 9695-9702.	1.8	1
77	Unexpected Electrochemical Behavior of Crown-Based Organic Compounds for Lithium-Ion Battery Cathodes. Industrial & Engineering Chemistry Research, 2021, 60, 7764-7774.	1.8	0
78	Unraveling Three-Stage Discharging Behaviors of Bio-Inspired Organic Cathode Materials (Adv. Funct.) Tj ETQq0,0,0 rgBT /Overlock 1	7.8	0
79	Modulation of Backbone Architecture to Design Structurally Durable Tetracyanoquinodimethane Derivatives with High Redox Activity. ACS Applied Energy Materials, 2022, 5, 7791-7801.	2.5	0