Kah Chun Lau

List of Publications by Year
in descending order

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81 papers	5,389 citations	109264 35 h-index	82499 72 g-index
88 all docs	88 docs citations	88 times ranked	5711 citing authors

#	Article	IF	Citations
1	First-Principles Study of Amorphous Al2O3 ALD Coating in Li-S Battery Electrode Design. Energies, 2022, 15, 390.	1.6	3
2	Machine-Learning Model Prediction of Ionic Liquids Melting Points. Applied Sciences (Switzerland), 2022, 12, 2408.	1.3	6
3	K⁺ Single Cation Ionic Liquids Electrolytes with Low Melting Asymmetric Salt. Journal of Physical Chemistry C, 2022, 126, 11407-11413.	1.5	8
4	Implication of Mechanical Properties of Li-S Binary Compounds Obtained from the First-Principles Study. Journal of Physical Chemistry C, 2021, 125, 290-294.	1.5	9
5	A XANES study of lithium polysulfide solids: a first-principles study. Materials Advances, 2021, 2, 6403-6410.	2.6	6
6	Two-Dimensional Nanomaterials as Anticorrosion Surface Coatings for Uranium Metal: Physical Insights from First-Principles Theory. ACS Applied Nano Materials, 2021, 4, 5038-5046.	2.4	4
7	Electronic properties of Ir3Li and ultra-nanocrystalline lithium superoxide formation. Nano Energy, 2021, 90, 106549.	8.2	3
8	Unusual Melting Trend in an Alkali Asymmetric Sulfonamide Salt Series: Single-Crystal Analysis and Modeling. Inorganic Chemistry, 2021, 60, 14679-14686.	1.9	5
9	Molecular Layer Deposition of Crosslinked Polymeric Lithicone for Superior Lithium Metal Anodes. Energy Material Advances, 2021, 2021, .	4.7	27
10	Highly stable potassium metal batteries enabled by regulating surface chemistry in ether electrolyte. Energy Storage Materials, 2021, 42, 526-532.	9.5	37
11	Computational study of the adsorption of bimetallic clusters on alumina substrate. Surface Science, 2020, 700, 121682.	0.8	2
12	Novel Metallic Crystalline Phase of Li2S3. Journal of Physical Chemistry C, 2019, 123, 28027-28034.	1.5	3
13	In Situ Formed Ir₃Li Nanoparticles as Active Cathode Material in Liâ€“Oxygen Batteries. Journal of Physical Chemistry A, 2019, 123, 10047-10056.	1.1	11
14	Artificial Solidâ€Electrolyte Interphase Enabled Highâ€Capacity and Stable Cycling Potassium Metal Batteries. Advanced Energy Materials, 2019, 9, 1902697.	10.2	81
15	Nitrogen-Doped Graphene on Copper: Edge-Guided Doping Process and Doping-Induced Variation of Local Work Function. Journal of Physical Chemistry C, 2019, 123, 8802-8812.	1.5	7
16	Microwave growth and tunable photoluminescence of nitrogen-doped graphene and carbon nitride quantum dots. Journal of Materials Chemistry C, 2019, 7, 5468-5476.	2.7	75
17	Thermodynamic and Mechanical Stability of Crystalline Phases of Li2S2. Journal of Physical Chemistry C, 2019, 123, 4674-4681.	1.5	16
18	Facet-dependent active sites of a single Cu2O particle photocatalyst for CO2 reduction to methanol. Nature Energy, 2019, 4, 957-968.	19.8	349

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19	Identification and Implications of Lithium Superoxide in Liâ€“O₂ Batteries. ACS Energy Letters, 2018, 3, 1105-1109.	8.8	47
20	A lithiumâ€“oxygen battery with a long cycle life in an air-like atmosphere. Nature, 2018, 555, 502-506.	13.7	433
21	Structureâ€“Property of Lithiumâ€“Sulfur Nanoparticles via Molecular Dynamics Simulation. ACS Applied Materials & Interfaces, 2018, 10, 37575-37585.	4.0	15
22	Exploring Stability of Nonaqueous Electrolytes for Potassium-Ion Batteries. ACS Applied Energy Materials, 2018, 1, 1828-1833.	2.5	78
23	Atomic and Molecular Layer Deposition for Superior Lithiumâ€Sulfur Batteries: Strategies, Performance, and Mechanisms. Batteries and Supercaps, 2018, 1, 41-68.	2.4	50
24	Lithium Superoxide Hydrolysis and Relevance to Liâ€“O₂ Batteries. Journal of Physical Chemistry C, 2017, 121, 9657-9661.	1.5	41
25	Mass and charge transport relevant to the formation of toroidal lithium peroxide nanoparticles in an aprotic lithium-oxygen battery: An experimental and theoretical modeling study. Nano Research, 2017, 10, 4327-4336.	5.8	12
26	Elucidating the Solvation Structure and Dynamics of Lithium Polysulfides Resulting from Competitive Salt and Solvent Interactions. Chemistry of Materials, 2017, 29, 3375-3379.	3.2	117
27	Dendrite-Free Potassiumâ€“Oxygen Battery Based on a Liquid Alloy Anode. ACS Applied Materials & Interfaces, 2017, 9, 31871-31878.	4.0	72
28	Computational Studies of Solubilities of LiO₂and Li₂O₂in Aprotic Solvents. Journal of the Electrochemical Society, 2017, 164, E3696-E3701.	1.3	26
29	Morse-Smale Analysis of Ion Diffusion in Ab Initio Battery Materials Simulations. Mathematics and Visualization, 2017, , 135-149.	0.4	3
30	Restricting the Solubility of Polysulfides in Liâ€S Batteries Via Electrolyte Salt Selection. Advanced Energy Materials, 2016, 6, 1600160.	10.2	66
31	Solvent Effects on Polysulfide Redox Kinetics and Ionic Conductivity in Lithium-Sulfur Batteries. Journal of the Electrochemical Society, 2016, 163, A3111-A3116.	1.3	74
32	Effect of Hydrofluoroether Cosolvent Addition on Li Solvation in Acetonitrile-Based Solvate Electrolytes and Its Influence on S Reduction in a Liâ€“S Battery. ACS Applied Materials & Interfaces, 2016, 8, 34360-34371.	4.0	58
33	Concentrated Electrolyte for the Sodiumâ€“Oxygen Battery: Solvation Structure and Improved Cycle Life. Angewandte Chemie, 2016, 128, 15536-15540.	1.6	20
34	Concentrated Electrolyte for the Sodiumâ€“Oxygen Battery: Solvation Structure and Improved Cycle Life. Angewandte Chemie - International Edition, 2016, 55, 15310-15314.	7.2	97
35	A lithiumâ€“oxygen battery based on lithium superoxide. Nature, 2016, 529, 377-382.	13.7	633
36	Interstitial and Interlayer Ion Diffusion Geometry Extraction in Graphitic Nanosphere Battery Materials. IEEE Transactions on Visualization and Computer Graphics, 2016, 22, 916-925.	2.9	19

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37	Microstructural Characterization of Air Electrode Architectures in Lithium-Oxygen Batteries. Microscopy and Microanalysis, 2015, 21, 1373-1374.	0.2	3
38	An atomistically informed mesoscale model for growth and coarsening during discharge in lithium-oxygen batteries. Journal of Chemical Physics, 2015, 143, 224113.	1.2	22
39	The Effect of Potassium Impurities Deliberately Introduced into Activated Carbon Cathodes on the Performance of Lithiumâ€“Oxygen Batteries. ChemSusChem, 2015, 8, 4235-4241.	3.6	13
40	Frontispiece: Implications of the Unpaired Spins in Li-O2Battery Chemistry and Electrochemistry: A Minireview. ChemPlusChem, 2015, 80, n/a-n/a.	1.3	0
41	Interfacial Effects on Lithium Superoxide Disproportionation in Li-O₂ Batteries. Nano Letters, 2015, 15, 1041-1046.	4.5	92
42	Theoretical Exploration of Various Lithium Peroxide Crystal Structures in a Li-Air Battery. Energies, 2015, 8, 529-548.	1.6	13
43	A Mo₂C/Carbon Nanotube Composite Cathode for Lithiumâ€“Oxygen Batteries with High Energy Efficiency and Long Cycle Life. ACS Nano, 2015, 9, 4129-4137.	7.3	207
44	Reviewâ€”Understanding and Mitigating Some of the Key Factors that Limit Non-Aqueous Lithium-Air Battery Performance. Journal of the Electrochemical Society, 2015, 162, A2439-A2446.	1.3	27
45	Implications of the Unpaired Spins in Liâ€“O₂ Battery Chemistry and Electrochemistry: A Minireview. ChemPlusChem, 2015, 80, 336-343.	1.3	17
46	Aprotic Electrolytes in Liâ€“Air Batteries. Modern Aspects of Electrochemistry, 2014, , 445-466.	0.2	0
47	Probing the evolution and morphology of hard carbon spheres. Carbon, 2014, 68, 104-111.	5.4	44
48	Investigation of the Decomposition Mechanism of Lithium Bis(oxalate)borate (LiBOB) Salt in the Electrolyte of an Aprotic Liâ€“O₂ Battery. Energy Technology, 2014, 2, 348-354.	1.8	13
49	Effect of the size-selective silver clusters on lithium peroxide morphology in lithiumâ€“oxygen batteries. Nature Communications, 2014, 5, 4895.	5.8	186
50	Understanding Side Reactions in Kâ€“O₂ Batteries for Improved Cycle Life. ACS Applied Materials & Interfaces, 2014, 6, 19299-19307.	4.0	117
51	Structure and Stability of Lithium Superoxide Clusters and Relevance to Liâ€“O₂ Batteries. Journal of Physical Chemistry Letters, 2014, 5, 813-819.	2.1	74
52	Raman Evidence for Late Stage Disproportionation in a Liâ€“O₂ Battery. Journal of Physical Chemistry Letters, 2014, 5, 2705-2710.	2.1	144
53	Atomistic and First Principles: Computational Studies of LiO2 Batteries. , 2014, , 159-177.		2
54	Compatibility of lithium salts with solvent of the non-aqueous electrolyte in Liâ€“O2 batteries. Physical Chemistry Chemical Physics, 2013, 15, 5572.	1.3	76

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55	Interactions of Dimethoxy Ethane with Li₂O₂ Clusters and Likely Decomposition Mechanisms for Liâ€“O₂ Batteries. Journal of Physical Chemistry C, 2013, 117, 8041-8049.	1.5	74
56	A nanostructured cathode architecture for low charge overpotential in lithium-oxygen batteries. Nature Communications, 2013, 4, 2383.	5.8	379
57	Disproportionation in Liâ€“O₂ Batteries Based on a Large Surface Area Carbon Cathode. Journal of the American Chemical Society, 2013, 135, 15364-15372.	6.6	282
58	Magnetism in Lithiumâ€“Oxygen Discharge Product. ChemSusChem, 2013, 6, 1196-1202.	3.6	23
59	Evidence for lithium superoxide-like species in the discharge product of a Liâ€“O2 battery. Physical Chemistry Chemical Physics, 2013, 15, 3764.	1.3	188
60	Electronic Structure of Lithium Peroxide Clusters and Relevance to Lithiumâ€“Air Batteries. Journal of Physical Chemistry C, 2012, 116, 23890-23896.	1.5	64
61	Density Functional Investigation of the Thermodynamic Stability of Lithium Oxide Bulk Crystalline Structures as a Function of Oxygen Pressure. Journal of Physical Chemistry C, 2011, 115, 23625-23633.	1.5	89
62	Molecular dynamics simulation of yttria-stabilized zirconia (YSZ) crystalline and amorphous solids. Journal of Physics Condensed Matter, 2011, 23, 035401.	0.7	39
63	Increased Stability Toward Oxygen Reduction Products for Lithium-Air Batteries with Oligoether-Functionalized Silane Electrolytes. Journal of Physical Chemistry C, 2011, 115, 25535-25542.	1.5	166
64	Kinetic Monte Carlo simulation of the elementary electrochemistry in a hydrogen-powered solid oxide fuel cell. Journal of Power Sources, 2010, 195, 4177-4184.	4.0	18
65	Kinetic Monte Carlo Simulation of AC Impedance on the Cathode Side of a Solid Oxide Fuel Cell. Journal of the Electrochemical Society, 2010, 157, B90.	1.3	4
66	Atomistic Modeling of Solid Oxide Fuel Cells. Annual Reports in Computational Chemistry, 2010, , 201-234.	0.9	2
67	Structure and stability of Mg-intercalated boron nanotubes and crystalline bundles. Journal of Physics Condensed Matter, 2009, 21, 045304.	0.7	8
68	Kinetic Monte Carlo simulation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si72.gif" display="inline" overflow="scroll"><mml:mrow><mml:msup><mml:mrow><mml:mtext>O</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:m incorporation in the yttria stabilized zirconia (YSZ) fuel cell. Chemical Physics Letters, 2009, 471, 326-330.	1.2	12
69	Lattice dielectric and thermodynamic properties of yttria stabilized zirconia solids. Journal of Physics Condensed Matter, 2009, 21, 145402.	0.7	14
70	Boron and Boron Carbide Materials: Nanostructures and Crystalline Solids. , 2009, , 271-291.		2
71	Kinetic Monte Carlo simulation of the Yttria Stabilized Zirconia (YSZ) fuel cell cathode. Solid State Ionics, 2008, 179, 1912-1920.	1.3	20
72	Thermodynamic Stability of Novel Boron Sheet Configurations. Journal of Physical Chemistry B, 2008, 112, 10217-10220.	1.2	41

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73	First-principles study of crystalline bundles of single-walled boron nanotubes with small diameter. Journal of Physics Condensed Matter, 2008, 20, 125202.	0.7	15
74	Stability and Electronic Properties of Atomistically-Engineered 2D Boron Sheets. Journal of Physical Chemistry C, 2007, 111, 2906-2912.	1.5	166
75	Theoretical study of electron transport in boron nanotubes. Applied Physics Letters, 2006, 88, 212111.	1.5	41
76	First-principles study of the stability and electronic properties of sheets and nanotubes of elemental boron. Chemical Physics Letters, 2006, 418, 549-554.	1.2	65
77	A theoretical study of vibrational properties of neutral and cationic B12 clusters. International Journal of Quantum Chemistry, 2005, 102, 656-664.	1.0	27
78	A theoretical study of electronic and vibrational properties of neutral, cationic, and anionic B24 clusters. International Journal of Quantum Chemistry, 2005, 103, 866-874.	1.0	28
79	The 2D-3D structural transition and chemical bonding in elemental boron nanoclusters. Computing Letters, 2005, 1, 259-270.	0.5	7
80	Equilibrium geometry and electron detachment energies of anionic Cr2O4, Cr2O5, and Cr2O6 clusters. Chemical Physics Letters, 2004, 393, 112-117.	1.2	16
81	Structure, Energetics, Electronic, and Hydration Properties of Neutral and Anionic Al3O6, Al3O7, and Al3O8 Clusters. Journal of Physical Chemistry A, 2004, 108, 5081-5090.	1.1	23