

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 | A lithium–oxygen battery based on lithium superoxide. <i>Nature</i> , 2016, 529, 377-382. | 13.7 | 633 |
| 2 | A lithium–oxygen battery with a long cycle life in an air-like atmosphere. <i>Nature</i> , 2018, 555, 502-506. | 13.7 | 433 |
| 3 | A nanostructured cathode architecture for low charge overpotential in lithium-oxygen batteries. <i>Nature Communications</i> , 2013, 4, 2383. | 5.8 | 379 |
| 4 | Facet-dependent active sites of a single Cu ₂ O particle photocatalyst for CO ₂ reduction to methanol. <i>Nature Energy</i> , 2019, 4, 957-968. | 19.8 | 349 |
| 5 | Disproportionation in Li–O ₂ Batteries Based on a Large Surface Area Carbon Cathode. <i>Journal of the American Chemical Society</i> , 2013, 135, 15364-15372. | 6.6 | 282 |
| 6 | A Mo ₂ C/Carbon Nanotube Composite Cathode for Lithium–Oxygen Batteries with High Energy Efficiency and Long Cycle Life. <i>ACS Nano</i> , 2015, 9, 4129-4137. | 7.3 | 207 |
| 7 | Evidence for lithium superoxide-like species in the discharge product of a Li–O ₂ battery. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 3764. | 1.3 | 188 |
| 8 | Effect of the size-selective silver clusters on lithium peroxide morphology in lithium–oxygen batteries. <i>Nature Communications</i> , 2014, 5, 4895. | 5.8 | 186 |
| 9 | Stability and Electronic Properties of Atomistically-Engineered 2D Boron Sheets. <i>Journal of Physical Chemistry C</i> , 2007, 111, 2906-2912. | 1.5 | 166 |
| 10 | Increased Stability Toward Oxygen Reduction Products for Lithium-Air Batteries with Oligoether-Functionalized Silane Electrolytes. <i>Journal of Physical Chemistry C</i> , 2011, 115, 25535-25542. | 1.5 | 166 |
| 11 | Raman Evidence for Late Stage Disproportionation in a Li–O ₂ Battery. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2705-2710. | 2.1 | 144 |
| 12 | Understanding Side Reactions in K–O ₂ Batteries for Improved Cycle Life. <i>ACS Applied Materials & Interfaces</i> , 2014, 6, 19299-19307. | 4.0 | 117 |
| 13 | Elucidating the Solvation Structure and Dynamics of Lithium Polysulfides Resulting from Competitive Salt and Solvent Interactions. <i>Chemistry of Materials</i> , 2017, 29, 3375-3379. | 3.2 | 117 |
| 14 | Concentrated Electrolyte for the Sodium–Oxygen Battery: Solvation Structure and Improved Cycle Life. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 15310-15314. | 7.2 | 97 |
| 15 | Interfacial Effects on Lithium Superoxide Disproportionation in Li–O ₂ Batteries. <i>Nano Letters</i> , 2015, 15, 1041-1046. | 4.5 | 92 |
| 16 | Density Functional Investigation of the Thermodynamic Stability of Lithium Oxide Bulk Crystalline Structures as a Function of Oxygen Pressure. <i>Journal of Physical Chemistry C</i> , 2011, 115, 23625-23633. | 1.5 | 89 |
| 17 | Artificial Solid–Electrolyte Interphase Enabled High–Capacity and Stable Cycling Potassium Metal Batteries. <i>Advanced Energy Materials</i> , 2019, 9, 1902697. | 10.2 | 81 |
| 18 | Exploring Stability of Nonaqueous Electrolytes for Potassium-Ion Batteries. <i>ACS Applied Energy Materials</i> , 2018, 1, 1828-1833. | 2.5 | 78 |

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|----|---|------|-----------|
| 19 | Compatibility of lithium salts with solvent of the non-aqueous electrolyte in Li ⁺ O ₂ batteries. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 5572. | 1.3 | 76 |
| 20 | Microwave growth and tunable photoluminescence of nitrogen-doped graphene and carbon nitride quantum dots. <i>Journal of Materials Chemistry C</i> , 2019, 7, 5468-5476. | 2.7 | 75 |
| 21 | Interactions of Dimethoxy Ethane with Li ₂ O ₂ Clusters and Likely Decomposition Mechanisms for Li ⁺ O ₂ Batteries. <i>Journal of Physical Chemistry C</i> , 2013, 117, 8041-8049. | 1.5 | 74 |
| 22 | Structure and Stability of Lithium Superoxide Clusters and Relevance to Li ⁺ O ₂ Batteries. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 813-819. | 2.1 | 74 |
| 23 | Solvent Effects on Polysulfide Redox Kinetics and Ionic Conductivity in Lithium-Sulfur Batteries. <i>Journal of the Electrochemical Society</i> , 2016, 163, A3111-A3116. | 1.3 | 74 |
| 24 | Dendrite-Free Potassium ⁺ Oxygen Battery Based on a Liquid Alloy Anode. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 31871-31878. | 4.0 | 72 |
| 25 | Restricting the Solubility of Polysulfides in Li ⁺ S Batteries Via Electrolyte Salt Selection. <i>Advanced Energy Materials</i> , 2016, 6, 1600160. | 10.2 | 66 |
| 26 | First-principles study of the stability and electronic properties of sheets and nanotubes of elemental boron. <i>Chemical Physics Letters</i> , 2006, 418, 549-554. | 1.2 | 65 |
| 27 | Electronic Structure of Lithium Peroxide Clusters and Relevance to Lithium ⁺ Air Batteries. <i>Journal of Physical Chemistry C</i> , 2012, 116, 23890-23896. | 1.5 | 64 |
| 28 | Effect of Hydrofluoroether Cosolvent Addition on Li Solvation in Acetonitrile-Based Solvate Electrolytes and Its Influence on S Reduction in a Li ⁺ S Battery. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 34360-34371. | 4.0 | 58 |
| 29 | Atomic and Molecular Layer Deposition for Superior Lithium ⁺ Sulfur Batteries: Strategies, Performance, and Mechanisms. <i>Batteries and Supercaps</i> , 2018, 1, 41-68. | 2.4 | 50 |
| 30 | Identification and Implications of Lithium Superoxide in Li ⁺ O ₂ Batteries. <i>ACS Energy Letters</i> , 2018, 3, 1105-1109. | 8.8 | 47 |
| 31 | Probing the evolution and morphology of hard carbon spheres. <i>Carbon</i> , 2014, 68, 104-111. | 5.4 | 44 |
| 32 | Theoretical study of electron transport in boron nanotubes. <i>Applied Physics Letters</i> , 2006, 88, 212111. | 1.5 | 41 |
| 33 | Thermodynamic Stability of Novel Boron Sheet Configurations. <i>Journal of Physical Chemistry B</i> , 2008, 112, 10217-10220. | 1.2 | 41 |
| 34 | Lithium Superoxide Hydrolysis and Relevance to Li ⁺ O ₂ Batteries. <i>Journal of Physical Chemistry C</i> , 2017, 121, 9657-9661. | 1.5 | 41 |
| 35 | Molecular dynamics simulation of yttria-stabilized zirconia (YSZ) crystalline and amorphous solids. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 035401. | 0.7 | 39 |
| 36 | Highly stable potassium metal batteries enabled by regulating surface chemistry in ether electrolyte. <i>Energy Storage Materials</i> , 2021, 42, 526-532. | 9.5 | 37 |

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|----|--|-----|-----------|
| 37 | A theoretical study of electronic and vibrational properties of neutral, cationic, and anionic B ₂₄ clusters. <i>International Journal of Quantum Chemistry</i> , 2005, 103, 866-874. | 1.0 | 28 |
| 38 | A theoretical study of vibrational properties of neutral and cationic B ₁₂ clusters. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 656-664. | 1.0 | 27 |
| 39 | Review—Understanding and Mitigating Some of the Key Factors that Limit Non-Aqueous Lithium-Air Battery Performance. <i>Journal of the Electrochemical Society</i> , 2015, 162, A2439-A2446. | 1.3 | 27 |
| 40 | Molecular Layer Deposition of Crosslinked Polymeric Lithicone for Superior Lithium Metal Anodes. <i>Energy Material Advances</i> , 2021, 2021, . | 4.7 | 27 |
| 41 | Computational Studies of Solubilities of LiO ₂ and Li ₂ O ₂ in Aprotic Solvents. <i>Journal of the Electrochemical Society</i> , 2017, 164, E3696-E3701. | 1.3 | 26 |
| 42 | Structure, Energetics, Electronic, and Hydration Properties of Neutral and Anionic Al ₃ O ₆ , Al ₃ O ₇ , and Al ₃ O ₈ Clusters. <i>Journal of Physical Chemistry A</i> , 2004, 108, 5081-5090. | 1.1 | 23 |
| 43 | Magnetism in Lithium—Oxygen Discharge Product. <i>ChemSusChem</i> , 2013, 6, 1196-1202. | 3.6 | 23 |
| 44 | An atomistically informed mesoscale model for growth and coarsening during discharge in lithium-oxygen batteries. <i>Journal of Chemical Physics</i> , 2015, 143, 224113. | 1.2 | 22 |
| 45 | Kinetic Monte Carlo simulation of the Yttria Stabilized Zirconia (YSZ) fuel cell cathode. <i>Solid State Ionics</i> , 2008, 179, 1912-1920. | 1.3 | 20 |
| 46 | Concentrated Electrolyte for the Sodium—Oxygen Battery: Solvation Structure and Improved Cycle Life. <i>Angewandte Chemie</i> , 2016, 128, 15536-15540. | 1.6 | 20 |
| 47 | Interstitial and Interlayer Ion Diffusion Geometry Extraction in Graphitic Nanosphere Battery Materials. <i>IEEE Transactions on Visualization and Computer Graphics</i> , 2016, 22, 916-925. | 2.9 | 19 |
| 48 | Kinetic Monte Carlo simulation of the elementary electrochemistry in a hydrogen-powered solid oxide fuel cell. <i>Journal of Power Sources</i> , 2010, 195, 4177-4184. | 4.0 | 18 |
| 49 | Implications of the Unpaired Spins in Li—O ₂ Battery Chemistry and Electrochemistry: A Minireview. <i>ChemPlusChem</i> , 2015, 80, 336-343. | 1.3 | 17 |
| 50 | Equilibrium geometry and electron detachment energies of anionic Cr ₂ O ₄ , Cr ₂ O ₅ , and Cr ₂ O ₆ clusters. <i>Chemical Physics Letters</i> , 2004, 393, 112-117. | 1.2 | 16 |
| 51 | Thermodynamic and Mechanical Stability of Crystalline Phases of Li ₂ S ₂ . <i>Journal of Physical Chemistry C</i> , 2019, 123, 4674-4681. | 1.5 | 16 |
| 52 | First-principles study of crystalline bundles of single-walled boron nanotubes with small diameter. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 125202. | 0.7 | 15 |
| 53 | Structure—Property of Lithium—Sulfur Nanoparticles via Molecular Dynamics Simulation. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 37575-37585. | 4.0 | 15 |
| 54 | Lattice dielectric and thermodynamic properties of yttria stabilized zirconia solids. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 145402. | 0.7 | 14 |

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|----|--|-----|-----------|
| 55 | Investigation of the Decomposition Mechanism of Lithium Bis(oxalate)borate (LiBOB) Salt in the Electrolyte of an Aprotic Li ⁺ O ₂ Battery. <i>Energy Technology</i> , 2014, 2, 348-354. | 1.8 | 13 |
| 56 | The Effect of Potassium Impurities Deliberately Introduced into Activated Carbon Cathodes on the Performance of Lithium ⁺ Oxygen Batteries. <i>ChemSusChem</i> , 2015, 8, 4235-4241. | 3.6 | 13 |
| 57 | Theoretical Exploration of Various Lithium Peroxide Crystal Structures in a Li-Air Battery. <i>Energies</i> , 2015, 8, 529-548. | 1.6 | 13 |
| 58 | 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. <i>Nano Research</i> , 2017, 10, 4327-4336. | 5.8 | 12 |
| 59 | Kinetic Monte Carlo simulation of $\frac{1}{2}$ O ₂ incorporation in the yttria stabilized zirconia (YSZ) fuel cell. <i>Chemical Physics Letters</i> , 2009, 471, 326-330. | 1.2 | 12 |
| 60 | In Situ Formed Ir ₃ Li Nanoparticles as Active Cathode Material in Li ⁺ Oxygen Batteries. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10047-10056. | 1.1 | 11 |
| 61 | Implication of Mechanical Properties of Li-S Binary Compounds Obtained from the First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2021, 125, 290-294. | 1.5 | 9 |
| 62 | Structure and stability of Mg-intercalated boron nanotubes and crystalline bundles. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 045304. | 0.7 | 8 |
| 63 | K ⁺ Single Cation Ionic Liquids Electrolytes with Low Melting Asymmetric Salt. <i>Journal of Physical Chemistry C</i> , 2022, 126, 11407-11413. | 1.5 | 8 |
| 64 | The 2D-3D structural transition and chemical bonding in elemental boron nanoclusters. <i>Computing Letters</i> , 2005, 1, 259-270. | 0.5 | 7 |
| 65 | Nitrogen-Doped Graphene on Copper: Edge-Guided Doping Process and Doping-Induced Variation of Local Work Function. <i>Journal of Physical Chemistry C</i> , 2019, 123, 8802-8812. | 1.5 | 7 |
| 66 | A XANES study of lithium polysulfide solids: a first-principles study. <i>Materials Advances</i> , 2021, 2, 6403-6410. | 2.6 | 6 |
| 67 | Machine-Learning Model Prediction of Ionic Liquids Melting Points. <i>Applied Sciences (Switzerland)</i> , 2022, 12, 2408. | 1.3 | 6 |
| 68 | Unusual Melting Trend in an Alkali Asymmetric Sulfonamide Salt Series: Single-Crystal Analysis and Modeling. <i>Inorganic Chemistry</i> , 2021, 60, 14679-14686. | 1.9 | 5 |
| 69 | Kinetic Monte Carlo Simulation of AC Impedance on the Cathode Side of a Solid Oxide Fuel Cell. <i>Journal of the Electrochemical Society</i> , 2010, 157, B90. | 1.3 | 4 |
| 70 | Two-Dimensional Nanomaterials as Anticorrosion Surface Coatings for Uranium Metal: Physical Insights from First-Principles Theory. <i>ACS Applied Nano Materials</i> , 2021, 4, 5038-5046. | 2.4 | 4 |
| 71 | Microstructural Characterization of Air Electrode Architectures in Lithium-Oxygen Batteries. <i>Microscopy and Microanalysis</i> , 2015, 21, 1373-1374. | 0.2 | 3 |
| 72 | Novel Metallic Crystalline Phase of Li ₂ S ₃ . <i>Journal of Physical Chemistry C</i> , 2019, 123, 28027-28034. | 1.5 | 3 |

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|----|--|-----|-----------|
| 73 | Electronic properties of Ir ₃ Li and ultra-nanocrystalline lithium superoxide formation. Nano Energy, 2021, 90, 106549. | 8.2 | 3 |
| 74 | Morse-Smale Analysis of Ion Diffusion in Ab Initio Battery Materials Simulations. Mathematics and Visualization, 2017, , 135-149. | 0.4 | 3 |
| 75 | First-Principles Study of Amorphous Al ₂ O ₃ ALD Coating in Li-S Battery Electrode Design. Energies, 2022, 15, 390. | 1.6 | 3 |
| 76 | Boron and Boron Carbide Materials: Nanostructures and Crystalline Solids. , 2009, , 271-291. | | 2 |
| 77 | Atomistic Modeling of Solid Oxide Fuel Cells. Annual Reports in Computational Chemistry, 2010, , 201-234. | 0.9 | 2 |
| 78 | Computational study of the adsorption of bimetallic clusters on alumina substrate. Surface Science, 2020, 700, 121682. | 0.8 | 2 |
| 79 | Atomistic and First Principles: Computational Studies of LiO ₂ Batteries. , 2014, , 159-177. | | 2 |
| 80 | Aprotic Electrolytes in Li-Air Batteries. Modern Aspects of Electrochemistry, 2014, , 445-466. | 0.2 | 0 |
| 81 | Frontispiece: Implications of the Unpaired Spins in Li-O ₂ Battery Chemistry and Electrochemistry: A Minireview. ChemPlusChem, 2015, 80, n/a-n/a. | 1.3 | 0 |