# Khoong Hong Khoo

List of Publications by Year
in descending order



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|---|---|---|---|
| 41 papers | 1,953 citations | 361413 20 h-index | 315739 38 g-index |
| 41 all docs | 41 docs citations | 41 times ranked | 3452 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Chemical affinity can govern notch-tip brittle-to-ductile transition in metallic glasses. Extreme Mechanics Letters, 2022, 52, 101651. | 4.1 | 5 |
| 2 | Tuning Damping and Magnetic Anisotropy in Ultrathin Boronâ€Engineered MgO/Coâ€“Feâ€“B/MgO Heterostructures. Advanced Electronic Materials, 2021, 7, 2100351. | 5.1 | 7 |
| 3 | Efficient Nearâ€Infrared Lightâ€Emitting Diodes based on In(Zn)Asâ€“In(Zn)Pâ€“GaPâ€“ZnS Quantum Dots. Advanced Functional Materials, 2020, 30, 1906483. | 14.9 | 28 |
| 4 | Thermodynamic Control in the Synthesis of Quantum-Confined Blue-Emitting CsPbBr<sub>3</sub> Perovskite Nanostrips. Journal of Physical Chemistry Letters, 2020, 11, 2036-2043. | 4.6 | 39 |
| 5 | First-principles study of coadsorption of Cu2+ and Clâ^' ions on the Cu (110) surface. RSC Advances, 2020, 10, 8212-8217. | 3.6 | 0 |
| 6 | Applying a machine learning interatomic potential to unravel theÂeffects of local lattice distortion on the elastic properties of multi-principal element alloys. Journal of Alloys and Compounds, 2019, 803, 1054-1062. | 5.5 | 41 |
| 7 | Color Patterning of Luminescent Perovskites via Lightâ€Mediated Halide Exchange with Haloalkanes. Advanced Materials, 2019, 31, e1901247. | 21.0 | 35 |
| 8 | Large-Stokes-Shifted Infrared-Emitting InAsâ€“In(Zn)Pâ€“ZnSeâ€“ZnS Giant-Shell Quantum Dots by One-Pot Continuous-Injection Synthesis. Chemistry of Materials, 2019, 31, 2019-2026. | 6.7 | 21 |
| 9 | Establishing new scaling relations on two-dimensional MXenes for CO<sub>2</sub> electroreduction. Journal of Materials Chemistry A, 2018, 6, 21885-21890. | 10.3 | 138 |
| 10 | Lead-free perovskite ceramics with ultraviolet-tunable optical and magnetic properties at room temperature. Journal of Applied Physics, 2018, 123, . | 2.5 | 2 |
| 11 | Computational Study of Al and Sc NMR Shielding in Metallic ScTâ€²Al Heusler Phases. Journal of Physical Chemistry C, 2017, 121, 12398-12406. | 3.1 | 5 |
| 12 | A perturbative DFT approach for magnetic anisotropy. Journal of Magnetism and Magnetic Materials, 2017, 428, 246-249. | 2.3 | 0 |
| 13 | Computational Study of Ga NMR Shielding in Metallic Gallides. Journal of Physical Chemistry C, 2017, 121, 753-760. | 3.1 | 16 |
| 14 | van der Waals Bonded Co/h-BN Contacts to Ultrathin Black Phosphorus Devices. Nano Letters, 2017, 17, 5361-5367. | 9.1 | 48 |
| 15 | Computational Study of Y NMR Shielding in Intermetallic Yttrium Compounds. Journal of Physical Chemistry C, 2017, 121, 28454-28461. | 3.1 | 2 |
| 16 | Helimagnetic order in bulk MnSi and CoSi/MnSi superlattices. Journal of Magnetism and Magnetic Materials, 2017, 421, 31-38. | 2.3 | 5 |
| 17 | Origin of Contact Resistance at Ferromagnetic Metalâ€“Graphene Interfaces. ACS Nano, 2016, 10, 11219-11227. | 14.6 | 16 |
| 18 | Graphene Nanomesh Formation by Fluorine Intercalation. Journal of Physical Chemistry C, 2015, 119, 29193-29200. | 3.1 | 15 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Low Resistance Metal Contacts to MoS<sub>2</sub> Devices with Nickel-Etched-Graphene Electrodes. ACS Nano, 2015, 9, 869-877. | 14.6 | 184 |
| 20 | Length dependence of electron transport through molecular wires â€“ a first principles perspective. Physical Chemistry Chemical Physics, 2015, 17, 77-96. | 2.8 | 46 |
| 21 | First-principles study of vibrational modes and Raman spectra in P-doped Si nanocrystals. Physical Review B, 2014, 89, . | 3.2 | 12 |
| 22 | Predictive DFT-Based Approaches to Charge and Spin Transport in Single-Molecule Junctions and Two-Dimensional Materials: Successes and Challenges. Accounts of Chemical Research, 2014, 47, 3250-3257. | 15.6 | 41 |
| 23 | Half metalâ†"semiconductor reversible switch in bimetallic sandwich molecular wire via redox reactions. Nano Energy, 2012, 1, 297-302. | 16.0 | 10 |
| 24 | Simulating liquid and amorphous silicon dioxide using real-space pseudopotentials. Physical Review B, 2012, 86, . | 3.2 | 15 |
| 25 | First-principles calculations of the magnetic anisotropic constants of Coâ€“Pd multilayers: Effect of stacking faults. Europhysics Letters, 2012, 99, 17001. | 2.0 | 6 |
| 26 | First-principles calculations of lattice-strained core-shell nanocrystals. Physical Review B, 2011, 84, . | 3.2 | 21 |
| 27 | Ab initiomolecular dynamics simulations of molten Al<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>Si<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>alloys. Physical Review B, 2011, 84, . | 3.2 | 17 |
| 28 | First-Principles Study of Confinement Effects on the Raman Spectra of Si Nanocrystals. Physical Review Letters, 2010, 105, 115504. | 7.8 | 58 |
| 29 | Ab initiomolecular dynamics simulations using a Chebyshev-filtered subspace iteration technique. Physical Review B, 2010, 82, . | 3.2 | 14 |
| 30 | Electron transport across carbon nanotube junctions decorated with Au nanoparticles: Density functional calculations. Physical Review B, 2009, 79, . | 3.2 | 22 |
| 31 | Negative Differential Resistance in Carbon Atomic Wire-Carbon Nanotube Junctions. Nano Letters, 2008, 8, 2900-2905. | 9.1 | 160 |
| 32 | Contact dependence of the conductance of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>molecular junctions from first principles. Physical Review B, 2008, 77, . | 3.2 | 12 |
| 33 | <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">K</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math>Monolayers for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mn>3</mml:mn><mml:mo>â‰¤</mml:mo><mml:mi>x</mml:mi><mml:mo>â‰¤</mml:mo><mml:mn>5</mml:mn></mml:math> | 7.8 | 31 |
| 34 | Electron transport and optical properties of carbon nanostructures from first principles. Computer Physics Communications, 2005, 169, 1-8. | 7.5 | 16 |
| 35 | Visualization of the Molecular Jahn-Teller Effect in an Insulating K4C60 Monolayer. Science, 2005, 310, 468-470. | 12.6 | 83 |
| 36 | Spatially Dependent Inelastic Tunneling in a Single Metallofullerene. Physical Review Letters, 2005, 94, 136802. | 7.8 | 64 |

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|---|---|---|---|
| 37 | Charge transfer and screening in individualC60molecules on metal substrates:â€ƒA scanning tunneling spectroscopy and theoretical study. Physical Review B, 2004, 70, . | 3.2 | 262 |
| 38 | Tuning the electronic properties of boron nitride nanotubes with transverse electric fields: A giant dc Stark effect. Physical Review B, 2004, 69, . | 3.2 | 256 |
| 39 | Spatially Mapping the Spectral Density of a SingleC60Molecule. Physical Review Letters, 2003, 90, 096802. | 7.8 | 191 |
| 40 | Mean-field renormalization group study of the long-range Ising model. Journal of Physics Condensed Matter, 2001, 13, 101-107. | 1.8 | 7 |
| 41 | Probing the Spin Hall Characteristics of W/CoFeB/MgO Based Heterostructures for Spinâ€Orbit Torque Based Magnetic Random Access Memory Application. Advanced Electronic Materials, 0, , 2100982. | 5.1 | 2 |