Khoong Hong Khoo

List of Publications by Year
in descending order

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	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
2	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
3	Spatially Mapping the Spectral Density of a SingleC60Molecule. Physical Review Letters, 2003, 90, 096802.	7.8	191
4	Low Resistance Metal Contacts to MoS₂ Devices with Nickel-Etched-Graphene Electrodes. ACS Nano, 2015, 9, 869-877.	14.6	184
5	Negative Differential Resistance in Carbon Atomic Wire-Carbon Nanotube Junctions. Nano Letters, 2008, 8, 2900-2905.	9.1	160
6	Establishing new scaling relations on two-dimensional MXenes for CO₂ electroreduction. Journal of Materials Chemistry A, 2018, 6, 21885-21890.	10.3	138
7	Visualization of the Molecular Jahn-Teller Effect in an Insulating K4C60 Monolayer. Science, 2005, 310, 468-470.	12.6	83
8	Spatially Dependent Inelastic Tunneling in a Single Metallofullerene. Physical Review Letters, 2005, 94, 136802.	7.8	64
9	First-Principles Study of Confinement Effects on the Raman Spectra of Si Nanocrystals. Physical Review Letters, 2010, 105, 115504.	7.8	58
10	van der Waals Bonded Co/h-BN Contacts to Ultrathin Black Phosphorus Devices. Nano Letters, 2017, 17, 5361-5367.	9.1	48
11	Length dependence of electron transport through molecular wires â€“ a first principles perspective. Physical Chemistry Chemical Physics, 2015, 17, 77-96.	2.8	46
12	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
13	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
14	Thermodynamic Control in the Synthesis of Quantum-Confined Blue-Emitting CsPbBr₃ Perovskite Nanostrips. Journal of Physical Chemistry Letters, 2020, 11, 2036-2043.	4.6	39
15	Color Patterning of Luminescent Perovskites via Lightâ€Mediated Halide Exchange with Haloalkanes. Advanced Materials, 2019, 31, e1901247.	21.0	35
16	Novel Orientational Ordering and Reentrant Metallicity in<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:m	7.8	31
17	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
18	Electron transport across carbon nanotube junctions decorated with Au nanoparticles: Density functional calculations. Physical Review B, 2009, 79, .	3.2	22

#	Article	IF	Citations
19	First-principles calculations of lattice-strained core-shell nanocrystals. Physical Review B, 2011, 84, .	3.2	21
20	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
21	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:mrow><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>alloys. Physical Review B, 2011, 84, .	3.2	17
22	Electron transport and optical properties of carbon nanostructures from first principles. Computer Physics Communications, 2005, 169, 1-8.	7.5	16
23	Origin of Contact Resistance at Ferromagnetic Metalâ€“Graphene Interfaces. ACS Nano, 2016, 10, 11219-11227.	14.6	16
24	Computational Study of Ga NMR Shielding in Metallic Gallides. Journal of Physical Chemistry C, 2017, 121, 753-760.	3.1	16
25	Simulating liquid and amorphous silicon dioxide using real-space pseudopotentials. Physical Review B, 2012, 86, .	3.2	15
26	Graphene Nanomesh Formation by Fluorine Intercalation. Journal of Physical Chemistry C, 2015, 119, 29193-29200.	3.1	15
27	Ab initiomolecular dynamics simulations using a Chebyshev-filtered subspace iteration technique. Physical Review B, 2010, 82, .	3.2	14
28	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
29	First-principles study of vibrational modes and Raman spectra in P-doped Si nanocrystals. Physical Review B, 2014, 89, .	3.2	12
30	Half metalâ†”semiconductor reversible switch in bimetallic sandwich molecular wire via redox reactions. Nano Energy, 2012, 1, 297-302.	16.0	10
31	Mean-field renormalization group study of the long-range Ising model. Journal of Physics Condensed Matter, 2001, 13, 101-107.	1.8	7
32	Tuning Damping and Magnetic Anisotropy in Ultrathin Boronâ€Engineered MgO/Coâ€“Feâ€“B/MgO Heterostructures. Advanced Electronic Materials, 2021, 7, 2100351.	5.1	7
33	First-principles calculations of the magnetic anisotropic constants of Coâ€“Pd multilayers: Effect of stacking faults. Europhysics Letters, 2012, 99, 17001.	2.0	6
34	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
35	Helimagnetic order in bulk MnSi and CoSi/MnSi superlattices. Journal of Magnetism and Magnetic Materials, 2017, 421, 31-38.	2.3	5
36	Chemical affinity can govern notch-tip brittle-to-ductile transition in metallic glasses. Extreme Mechanics Letters, 2022, 52, 101651.	4.1	5

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37	Computational Study of Y NMR Shielding in Intermetallic Yttrium Compounds. Journal of Physical Chemistry C, 2017, 121, 28454-28461.	3.1	2
38	Lead-free perovskite ceramics with ultraviolet-tunable optical and magnetic properties at room temperature. Journal of Applied Physics, 2018, 123, .	2.5	2
39	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
40	A perturbative DFT approach for magnetic anisotropy. Journal of Magnetism and Magnetic Materials, 2017, 428, 246-249.	2.3	0
41	First-principles study of coadsorption of Cu2+ and Clâ^' ions on the Cu (110) surface. RSC Advances, 2020, 10, 8212-8217.	3.6	0