# Eâ€j Kan

List of Publications by Year
in descending order

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| 160 | 8,300 | 53660 | 51492 |
|---|---|---|---|
| papers | citations | 45 h-index | 86 g-index |

| 165 | 165 | 165 | 9402 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Room-temperature Ferroelectricity in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>1</mml:mn><mml:msup><mml:mrow><mml:mi mathvariant="normal">T</mml:mi></mml:mrow><mml:mrow><mml:mo>â€²</mml:mo></mml:mrow></mml:msup></mml:mrow></mml:math> - <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>ReS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Multilayers. Physical Review Letters, 2022, 128, 067601. | 2.9 | 52 |
| 2 | Enabling High Loading in Singleâ€Atom Catalysts on Bare Substrate with Chemical Scissors by Saturating the Anchoring Sites. Small, 2022, 18, e2200073. | 5.2 | 14 |
| 3 | Popcorn-like Co<sub>3</sub>O<sub>4</sub> nanoparticles confined in a three-dimensional hierarchical N-doped carbon nanotube network as a highly-efficient trifunctional electrocatalyst for zincâ€“air batteries and water splitting devices. Inorganic Chemistry Frontiers, 2022, 9, 2517-2529. | 3.0 | 18 |
| 4 | Enabling High Loading in Singleâ€Atom Catalysts on Bare Substrate with Chemical Scissors by Saturating the Anchoring Sites (Small 19/2022). Small, 2022, 18, . | 5.2 | 2 |
| 5 | Toward Room-Temperature Electrical Control of Magnetic Order in Multiferroic van der Waals Materials. Nano Letters, 2022, 22, 5191-5197. | 4.5 | 25 |
| 6 | Ru Colloidosome Catalysts for the Hydrogen Oxidation Reaction in Alkaline Media. Journal of the American Chemical Society, 2022, 144, 11138-11147. | 6.6 | 47 |
| 7 | Substitutionally Dispersed Highâ€Oxidation CoO<sub>x</sub> Clusters in the Lattice of Rutile TiO<sub>2</sub> Triggering Efficient Coï£¿Ti Cooperative Catalytic Centers for Oxygen Evolution Reactions. Advanced Functional Materials, 2021, 31, 2009610. | 7.8 | 82 |
| 8 | Selective Construction of Magic Hierarchical Metalâ€“Organic Clusters on Surfaces. Journal of Physical Chemistry C, 2021, 125, 358-365. | 1.5 | 8 |
| 9 | Transition between half-metal and ferromagnetic semiconductor induced by silicon vacancy in bulk non-metallic substrate supported silicene. Journal Physics D: Applied Physics, 2021, 54, 125302. | 1.3 | 0 |
| 10 | Two-dimensional metal-free boron chalcogenides B<sub>2</sub>X<sub>3</sub> (X = Se and Te) as photocatalysts for water splitting under visible light. Nanoscale, 2021, 13, 3627-3632. | 2.8 | 9 |
| 11 | Dimension effect on ferroelectricity: a first-principles study on GeS nanoribbons. Physical Chemistry Chemical Physics, 2021, 23, 18863-18868. | 1.3 | 3 |
| 12 | Built-in electric field control of magnetic coupling in van der Waals semiconductors. Physical Review B, 2021, 103, . | 1.1 | 19 |
| 13 | Modulation on the Iron Centers by Selective Synthesis of Organic Ligands with Stereoâ€Specific Conformations. Small, 2021, 17, e2008036. | 5.2 | 2 |
| 14 | Controllable vdW Contacts between the Ferroelectric In<sub>2</sub>Se<sub>3</sub> Monolayer and Two-Dimensional Metals. Journal of Physical Chemistry C, 2021, 125, 10738-10746. | 1.5 | 21 |
| 15 | High-Temperature p-Orbital Half-Metallicity and Out-of-Plane Piezoelectricity in a GaN Monolayer Induced by Superhalogens. Journal of Physical Chemistry C, 2021, 125, 10027-10033. | 1.5 | 9 |
| 16 | Trimetallic Octahedral Niâ€“Coâ€“W Phosphoxide Sprouted from Plasma-Defect-Engineered Niâ€“Co Support for Ultrahigh-Performance Electrocatalytic Hydrogen Evolution. ACS Sustainable Chemistry and Engineering, 2021, 9, 7454-7465. | 3.2 | 21 |
| 17 | Nature of spin-lattice coupling in two-dimensional CrI3 and CrGeTe3. Science China: Physics, Mechanics and Astronomy, 2021, 64, 1. | 2.0 | 12 |
| 18 | Graphene-mediated ferromagnetic coupling in the nickel nano-islands/graphene hybrid. Science Advances, 2021, 7, . | 4.7 | 12 |

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| 19 | Improved contact properties of graphene-metal hybrid interfaces by grain boundaries. Applied Surface Science, 2021, 563, 150392. | 3.1 | 0 |
| 20 | Manipulating the Raman scattering rotation via magnetic field in an MoS2 monolayer. RSC Advances, 2021, 11, 4035-4041. | 1.7 | 2 |
| 21 | High-throughput calculations of spintronic tetra-phase transition metal dinitrides. Journal of Materials Chemistry C, 2021, 9, 14401-14407. | 2.7 | 8 |
| 22 | Unconventional distortion induced two-dimensional multiferroicity in a CrO<sub>3</sub> monolayer. Nanoscale, 2021, 13, 13048-13056. | 2.8 | 7 |
| 23 | Giant Biquadratic Exchange in 2D Magnets and Its Role in Stabilizing Ferromagnetism of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>NiCl</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></ Monolayers. Physical Review Letters, 2021, 127, 247204. | 2.9 | 31 |
| 24 | Discovery of twin orbital-order phases in ferromagnetic semiconducting VI<sub>3</sub> monolayer. Physical Chemistry Chemical Physics, 2020, 22, 512-517. | 1.3 | 29 |
| 25 | Tunable ferroelectric single-atom catalysis of CO oxidation using a Pt/In<sub>2</sub>Se<sub>3</sub> monolayer. Journal of Materials Chemistry A, 2020, 8, 20725-20731. | 5.2 | 17 |
| 26 | Water-sprouted, plasma-enhanced Ni-Co phospho-nitride nanosheets boost electrocatalytic hydrogen and oxygen evolution. Chemical Engineering Journal, 2020, 402, 126257. | 6.6 | 60 |
| 27 | Tuning Electronic and Magnetic Properties of Two-Dimensional Ferromagnetic Semiconductor CrI<sub>3</sub> through Adsorption of Benzene. Journal of Physical Chemistry C, 2020, 124, 22143-22149. | 1.5 | 20 |
| 28 | Surface-sensitive magnetic characterization technique for ultrathin ferromagnetic film with perpendicular magnetic anisotropy. AIP Advances, 2020, 10, 065019. | 0.6 | 1 |
| 29 | Prediction of room-temperature ferromagnetism in a two-dimensional direct band gap semiconductor. Nanoscale, 2020, 12, 15670-15676. | 2.8 | 38 |
| 30 | Electrical Control of Magnetic Phase Transition in a Type-I Multiferroic Double-Metal Trihalide Monolayer. Physical Review Letters, 2020, 124, 067602. | 2.9 | 84 |
| 31 | Switchable encapsulation of polysulfides in the transition between sulfur and lithium sulfide. Nature Communications, 2020, 11, 845. | 5.8 | 92 |
| 32 | Giant Band Gap Reduction and Insulatorâ€“Metal Transition in Two-Dimensional InX (X = Cl, Br, I) Layers. Journal of Physical Chemistry C, 2019, 123, 21763-21767. | 1.5 | 5 |
| 33 | Hydrogen Induced Etching Features of Wrinkled Graphene Domains. Nanomaterials, 2019, 9, 930. | 1.9 | 4 |
| 34 | Substrate-induced half-metallic property in epitaxial silicene. Europhysics Letters, 2019, 126, 57006. | 0.7 | 1 |
| 35 | Ultra-High-Temperature Ferromagnetism in Intrinsic Tetrahedral Semiconductors. Journal of the American Chemical Society, 2019, 141, 12413-12418. | 6.6 | 44 |
| 36 | Boosting the high-capacity with multi-active centers: A first-principles investigation of NiPS3 monolayer as an anode material. Applied Surface Science, 2019, 495, 143534. | 3.1 | 15 |

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| 37 | Boosting the Curie Temperature of Two-Dimensional Semiconducting CrI<sub>3</sub> Monolayer through van der Waals Heterostructures. Journal of Physical Chemistry C, 2019, 123, 17987-17993. | 1.5 | 74 |
| 38 | The Janus structures of group-III chalcogenide monolayers as promising photocatalysts for water splitting. Applied Surface Science, 2019, 478, 522-531. | 3.1 | 78 |
| 39 | Quinone-Facilitated Coordinated Bipyrene and Polypyrene on Au(111) by Capture of Gold Adatoms. Journal of Physical Chemistry C, 2019, 123, 16281-16287. | 1.5 | 8 |
| 40 | High-Temperature Ferromagnetism in an Fe<sub>3</sub>P Monolayer with a Large Magnetic Anisotropy. Journal of Physical Chemistry Letters, 2019, 10, 2733-2738. | 2.1 | 79 |
| 41 | Computational Dissection of 2D SiC<sub>7</sub> Monolayer: A Direct Band Gap Semiconductor and High Power Conversion Efficiency. Advanced Theory and Simulations, 2019, 2, 1900058. | 1.3 | 13 |
| 42 | Room-temperature magnetism and tunable energy gaps in edge-passivated zigzag graphene quantum dots. Npj 2D Materials and Applications, 2019, 3, . | 3.9 | 25 |
| 43 | Mechanical, Electronic, and Magnetic Properties of NiX<sub>2</sub> (X = Cl, Br, I) Layers. ACS Omega, 2019, 4, 5714-5721. | 1.6 | 40 |
| 44 | First-Principles Prediction of Room-Temperature Ferromagnetic Semiconductor MnS<sub>2</sub> via Isovalent Alloying. Journal of Physical Chemistry C, 2019, 123, 10114-10119. | 1.5 | 33 |
| 45 | Accurate K-edge X-ray photoelectron and absorption spectra of g-C<sub>3</sub>N<sub>4</sub> nanosheets by first-principles simulations and reinterpretations. Physical Chemistry Chemical Physics, 2019, 21, 22819-22830. | 1.3 | 70 |
| 46 | Progress and prospects in lowâ€dimensional multiferroic materials. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1409. | 6.2 | 53 |
| 47 | Band structure tuning and charge separation of MNX monolayers and MNX/GaS van der Waals heterostructures. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 108, 44-52. | 1.3 | 2 |
| 48 | Effect of Coulomb Correlation on the Magnetic Properties of Mn Clusters. Journal of Physical Chemistry A, 2018, 122, 4350-4356. | 1.1 | 4 |
| 49 | Ultrathin molybdenum disulfide/carbon nitride nanosheets with abundant active sites for enhanced hydrogen evolution. Nanoscale, 2018, 10, 1766-1773. | 2.8 | 57 |
| 50 | Designing half-metallic ferromagnetism by a new strategy: an example of superhalogen modified graphitic C<sub>3</sub>N<sub>4</sub>. Journal of Materials Chemistry C, 2018, 6, 1709-1714. | 2.7 | 21 |
| 51 | Prediction of Intrinsic Ferromagnetic Ferroelectricity in a Transition-Metal Halide Monolayer. Physical Review Letters, 2018, 120, 147601. | 2.9 | 217 |
| 52 | Atomically dispersed tungsten on metal halide monolayer as a ferromagnetic Chern insulator. Physical Review B, 2018, 98, . | 1.1 | 5 |
| 53 | Efficient Carrier Separation and Band Structure Tuning of Two-Dimensional C<sub>2</sub>N/GaTe van der Waals Heterostructure. Journal of Physical Chemistry C, 2018, 122, 15892-15902. | 1.5 | 55 |
| 54 | Hexagonal Boron Nitrideâ€“Metal Junction: Removing the Schottky Barriers by Grain Boundary. Advanced Theory and Simulations, 2018, 1, 1800045. | 1.3 | 5 |

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| 55 | Atomically thin mononitrides SiN and GeN: New two-dimensional wide band gap semiconductors. Europhysics Letters, 2018, 122, 47002. | 0.7 | 5 |
| 56 | Synthesis of Amorphous Carbon Film in Ethanol Inverse Diffusion Flames. Nanomaterials, 2018, 8, 656. | 1.9 | 4 |
| 57 | Toward Intrinsic Room-Temperature Ferromagnetism in Two-Dimensional Semiconductors. Journal of the American Chemical Society, 2018, 140, 11519-11525. | 6.6 | 280 |
| 58 | Band gap engineering and visible light response for GaS monolayer by isovalent anion-cation codoping. Materials Chemistry and Physics, 2017, 198, 275-282. | 2.0 | 19 |
| 59 | Van der Waals bilayer antimonene: A promising thermophotovoltaic cell material with 31% energy conversion efficiency. Nano Energy, 2017, 38, 561-568. | 8.2 | 92 |
| 60 | Stabilization of the Metastable Lead Iodide Perovskite Phase via Surface Functionalization. Nano Letters, 2017, 17, 4405-4414. | 4.5 | 204 |
| 61 | Quantum anomalous Hall effect in ferromagnetic transition metal halides. Physical Review B, 2017, 95, . | 1.1 | 110 |
| 62 | Edge-Modified Graphene Nanoribbons: Appearance of Robust Spiral Magnetism. Journal of Physical Chemistry C, 2017, 121, 1371-1376. | 1.5 | 12 |
| 63 | Prediction of another semimetallic silicene allotrope with Dirac fermions. Physics Letters, Section A: General, Atomic and Solid State Physics, 2017, 381, 3754-3759. | 0.9 | 31 |
| 64 | Semiconducting Groupâ€…15 Monolayers: A Broad Range of Band Gaps and High Carrier Mobilities. Angewandte Chemie, 2016, 128, 1698-1701. | 1.6 | 315 |
| 65 | Half-metallicity obtained in silicene nanosheet by nitrogenation engineering. Journal of Applied Physics, 2016, 120, 234303. | 1.1 | 9 |
| 66 | Quantum Phase Transition in Germanene and Stanene Bilayer: From Normal Metal to Topological Insulator. Journal of Physical Chemistry Letters, 2016, 7, 1919-1924. | 2.1 | 33 |
| 67 | Valley contrasting in epitaxial growth of In/Tl homoatomic monolayer with anomalous Nernst conductance. Physical Review B, 2016, 94, . | 1.1 | 7 |
| 68 | Theoretical realization of half-metallicity in two-dimensional monolayered molybdenum dinitride by Mo vacancy tuning. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 2669-2673. | 0.9 | 4 |
| 69 | A promising two-dimensional channel material: monolayer antimonide phosphorus. Science China Materials, 2016, 59, 648-656. | 3.5 | 28 |
| 70 | High-capacity hydrogen storage in Li-adsorbed g-C3N4. Materials Chemistry and Physics, 2016, 180, 440-444. | 2.0 | 21 |
| 71 | Realizing half-metallicity in K<sub>2</sub>CoF<sub>4</sub> exfoliated nanosheets via defect engineering. Physical Chemistry Chemical Physics, 2016, 18, 15765-15773. | 1.3 | 3 |
| 72 | Superhalogens as building blocks of two-dimensional organicâ€“inorganic hybrid perovskites for optoelectronics applications. Nanoscale, 2016, 8, 17836-17842. | 2.8 | 34 |

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| 73 | Cobalt Sulfide/Graphene Composite Hydrogel as Electrode for High-Performance Pseudocapacitors. Scientific Reports, 2016, 6, 21717. | 1.6 | 105 |
| 74 | New Ferroelectric Phase in Atomic-Thick Phosphorene Nanoribbons: Existence of in-Plane Electric Polarization. Nano Letters, 2016, 16, 8015-8020. | 4.5 | 55 |
| 75 | Electride: from computational characterization to theoretical design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 430-440. | 6.2 | 41 |
| 76 | Semiconducting Groupâ€…15 Monolayers: A Broad Range of Band Gaps and High Carrier Mobilities. Angewandte Chemie - International Edition, 2016, 55, 1666-1669. | 7.2 | 651 |
| 77 | Magnetic structure of (C5H12N)CuBr3: origin of the uniform Heisenberg chain behavior and the magnetic anisotropy of the Cu2+(S = 1/2) ions. RSC Advances, 2016, 6, 22722-22727. | 1.7 | 4 |
| 78 | Coexistence of metallic and insulating-like states in graphene. Scientific Reports, 2015, 5, 8974. | 1.6 | 3 |
| 79 | Two-dimensional silicon monolayers generated on c-BN(111) substrate. Physical Chemistry Chemical Physics, 2015, 17, 15694-15700. | 1.3 | 10 |
| 80 | Magnetic and electronic properties of frustrated spin dimer compound K2Fe2B2O7: A first-principles calculation. Solid State Communications, 2015, 220, 77-80. | 0.9 | 0 |
| 81 | Electronic and magnetic properties of an AlN monolayer doped with first-row elements: a first-principles study. RSC Advances, 2015, 5, 18352-18358. | 1.7 | 50 |
| 82 | Theoretical Prediction of Phosphorene and Nanoribbons As Fast-Charging Li Ion Battery Anode Materials. Journal of Physical Chemistry C, 2015, 119, 6923-6928. | 1.5 | 96 |
| 83 | Theoretical understanding of magnetic and electronic structures of Ti3C2 monolayer and its derivatives. Solid State Communications, 2015, 222, 9-13. | 0.9 | 41 |
| 84 | A promising way to open an energy gap in bilayer graphene. Nanoscale, 2015, 7, 17096-17101. | 2.8 | 13 |
| 85 | Vacancy-induced insulator â€“ direct spin gapless semiconductor â€“ half-metal transition in double perovskite La2CrFeO6: A first-principles study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2015, 379, 2897-2901. | 0.9 | 8 |
| 86 | Atomically Thin Transition-Metal Dinitrides: High-Temperature Ferromagnetism and Half-Metallicity. Nano Letters, 2015, 15, 8277-8281. | 4.5 | 168 |
| 87 | A theoretical study on the structural and physical properties of the ground-state CaC. Solid State Communications, 2015, 203, 10-15. | 0.9 | 2 |
| 88 | XiangetÂal.Reply:. Physical Review Letters, 2014, 112, 199802. | 2.9 | 3 |
| 89 | The effect of biaxial mechanical strain on the physical properties of double perovskite Sr2FeMoO6: A theoretical study. Solid State Communications, 2014, 191, 70-75. | 0.9 | 21 |
| 90 | Will a graphitic-like ZnO single-layer be an ideal substrate for graphene?. RSC Advances, 2014, 4, 17478. | 1.7 | 16 |

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| 91 | A Bâ€“Câ€“N hybrid porous sheet: an efficient metal-free visible-light absorption material. Physical Chemistry Chemical Physics, 2014, 16, 4299. | 1.3 | 13 |
| 92 | A promising monolayer membrane for oxygen separation from harmful gases: nitrogen-substituted polyphenylene. Nanoscale, 2014, 6, 9960-9964. | 2.8 | 51 |
| 93 | Ferroelectric-like structural transition in metallic LiOsO3. RSC Advances, 2014, 4, 26843. | 1.7 | 7 |
| 94 | Sandwich-structured MnO<sub>2</sub>/polypyrrole/reduced graphene oxide hybrid composites for high-performance supercapacitors. RSC Advances, 2014, 4, 9898-9904. | 1.7 | 113 |
| 95 | Improved permeability and selectivity in porous graphene for hydrogen purification. Physical Chemistry Chemical Physics, 2014, 16, 25755-25759. | 1.3 | 39 |
| 96 | Electronic properties and hydrogen storage application of designed porous nanotubes from a polyphenylene network. International Journal of Hydrogen Energy, 2014, 39, 18966-18975. | 3.8 | 33 |
| 97 | Theoretical study of CO oxidation on cationic, neutral, and anionic AuM dimers (M = Pd and Ag). Journal of Molecular Modeling, 2014, 20, 2313. | 0.8 | 4 |
| 98 | The effect of oxygen vacancy on the half-metallic nature of double perovskite Sr2FeMoO6: A theoretical study. Solid State Communications, 2014, 177, 57-60. | 0.9 | 22 |
| 99 | MnO2 Nanorods Intercalating Graphene Oxide/Polyaniline Ternary Composites for Robust High-Performance Supercapacitors. Scientific Reports, 2014, 4, 4824. | 1.6 | 215 |
| 100 | Tunable band gap and hydrogen adsorption property of a two-dimensional porous polymer by nitrogen substitution. Physical Chemistry Chemical Physics, 2013, 15, 666-670. | 1.3 | 20 |
| 101 | High-temperature ferro-electricity in two-dimensional atomic crystal. Applied Physics Letters, 2013, 103, . | 1.5 | 30 |
| 102 | Stability of graphitic-like zinc oxide layers under carriers doping: a first-principles study. Nanoscale, 2013, 5, 12111. | 2.8 | 10 |
| 103 | Boron-substituted graphyne as a versatile material with high storage capacities of Li and H2: a multiscale theoretical study. Physical Chemistry Chemical Physics, 2013, 15, 16120. | 1.3 | 96 |
| 104 | The strain effect on colossal oxygen ionic conductivity in nanoscale zirconia electrolytes: a first-principles-based study. Physical Chemistry Chemical Physics, 2013, 15, 2692. | 1.3 | 19 |
| 105 | Two-Dimensional Hexagonal Transition-Metal Oxide for Spintronics. Journal of Physical Chemistry Letters, 2013, 4, 1120-1125. | 2.1 | 58 |
| 106 | d0 magnetism in semiconductors through confining delocalized atomic orbitals. Applied Physics Letters, 2013, 102, 022422. | 1.5 | 10 |
| 107 | Towards Direct-Gap Silicon Phases by the Inverse Band Structure Design Approach. Physical Review Letters, 2013, 110, 118702. | 2.9 | 136 |
| 108 | Catenated metal-organic frameworks: Promising hydrogen purification materials and high hydrogen storage medium with further lithium doping. International Journal of Hydrogen Energy, 2013, 38, 9811-9818. | 3.8 | 37 |

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| 109 | Geometric and Electronic Structures as well as Thermodynamic Stability of Hexyl-Modified Silicon Nanosheet. Journal of Physical Chemistry C, 2013, 117, 13283-13288. | 1.5 | 16 |
| 110 | Influences of lithium doping and fullerene impregnation on hydrogen storage in metal organic frameworks. Molecular Simulation, 2013, 39, 968-974. | 0.9 | 12 |
| 111 | Stabilizing intrinsic defects in SnO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2013, 87, . | 1.1 | 40 |
| 112 | Carrier-tunable magnetism of graphene with single-atom vacancy. Journal of Applied Physics, 2013, 113, 213709. | 1.1 | 7 |
| 113 | Biaxial strain effect on the electronic and magnetic phase transitions in double perovskite La2FeMnO6: A first-principles study. Journal of Applied Physics, 2013, 114, . | 1.1 | 23 |
| 114 | First-principles investigations on the magnetic structure of Î±-NaMnO<sub>2</sub>. Journal of Physics Condensed Matter, 2012, 24, 456002. | 0.7 | 5 |
| 115 | Enhancing magnetic vacancies in semiconductors by strain. Applied Physics Letters, 2012, 100, 072401. | 1.5 | 21 |
| 116 | Two-dimensional organometallic porous sheets with possible high-temperature ferromagnetism. Nanoscale, 2012, 4, 5304. | 2.8 | 23 |
| 117 | Visible-Light-Absorption in Graphitic C<sub>3</sub>N<sub>4</sub> Bilayer: Enhanced by Interlayer Coupling. Journal of Physical Chemistry Letters, 2012, 3, 3330-3334. | 2.1 | 138 |
| 118 | Spin Reorientation in the Square-Lattice Antiferromagnets RMnAsO (R = Ce, Nd): Density Functional Analysis of the Spin-Exchange Interactions between the Rare-Earth and Transition-Metal Ions. Inorganic Chemistry, 2012, 51, 6890-6897. | 1.9 | 19 |
| 119 | Half-Metallicity in Organic Single Porous Sheets. Journal of the American Chemical Society, 2012, 134, 5718-5721. | 6.6 | 101 |
| 120 | Prominently Improved Hydrogen Purification and Dispersive Metal Binding for Hydrogen Storage by Substitutional Doping in Porous Graphene. Journal of Physical Chemistry C, 2012, 116, 21291-21296. | 1.5 | 76 |
| 121 | Unzipping carbon nanotubes into nanoribbons upon oxidation: A first-principles study. Nanoscale, 2012, 4, 1254. | 2.8 | 17 |
| 122 | Why the Band Gap of Graphene Is Tunable on Hexagonal Boron Nitride. Journal of Physical Chemistry C, 2012, 116, 3142-3146. | 1.5 | 103 |
| 123 | Tunable Magnetism in a Nonmetal-Substituted ZnO Monolayer: A First-Principles Study. Journal of Physical Chemistry C, 2012, 116, 11336-11342. | 1.5 | 180 |
| 124 | Site-selected doping in silicon nanowires by an external electric field. Nanoscale, 2011, 3, 3620. | 2.8 | 3 |
| 125 | Half-Metallic Dirac Point in B-Edge Hydrogenated BN Nanoribbons. Journal of Physical Chemistry C, 2011, 115, 17252-17254. | 1.5 | 38 |
| 126 | Single-ion anisotropy, Dzyaloshinskii-Moriya interaction, and negative magnetoresistance of the spin-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mfrac><mml:mrow><mml:mn>1</mml:mn></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:mfrac></mml:mrow></mml:math> xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>R</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Physical Review B, 2011, 83, . | 1.1 | 39 |

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| 127 | On the High Magnetic-Ordering Temperature of the 5d Magnetic Oxide Ca<sub>3</sub>LiOsO<sub>6</sub> Crystallizing in a Trigonal Crystal Structure: Density Functional Analysis. Inorganic Chemistry, 2011, 50, 4182-4186. | 1.9 | 11 |
| 128 | Lithium-doped MOF impregnated with lithium-coated fullerenes: A hydrogen storage route for high gravimetric and volumetric uptakes at ambient temperatures. Chemical Communications, 2011, 47, 7698. | 2.2 | 60 |
| 129 | Density Functional Theory Analysis of the Interplay between Jahnâ^'Teller Instability, Uniaxial Magnetism, Spin Arrangement, Metalâ^'Metal Interaction, and Spinâ^'Orbit Coupling in Ca<sub>3</sub>CoMO<sub>6</sub> (M = Co, Rh, Ir). Inorganic Chemistry, 2011, 50, 1758-1766. | 1.9 | 25 |
| 130 | Density Functional Investigation of the Difference in the Magnetic Structures of the Layered Triangular Antiferromagnets CuFeO2and AgCrO2. Chemistry of Materials, 2011, 23, 4181-4185. | 3.2 | 8 |
| 131 | Density functional predictions of new silicon allotropes: Electronic properties and potential applications to Li-battery anode materials. Solid State Communications, 2011, 151, 1228-1230. | 0.9 | 19 |
| 132 | Predicting the spin-lattice order of frustrated systems from first principles. Physical Review B, 2011, 84, . | 1.1 | 262 |
| 133 | General Theory for the Ferroelectric Polarization Induced by Spin-Spiral Order. Physical Review Letters, 2011, 107, 157202. | 2.9 | 100 |
| 134 | Thermodynamically stable single-side hydrogenated graphene. Physical Review B, 2010, 82, . | 1.1 | 47 |
| 135 | Ferroelectricity in Perovskites with s<sup>0</sup> Aâ€Site Cations: Toward Nearâ€Roomâ€Temperature Multiferroics. Angewandte Chemie - International Edition, 2010, 49, 1603-1606. | 7.2 | 22 |
| 136 | Ferrimagnetism in zigzag graphene nanoribbons induced by main-group adatoms. Applied Physics Letters, 2010, 96, . | 1.5 | 39 |
| 137 | Electrical rectification by selective wave-function coupling in small Ag clusters on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Si</mml:mtext><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mn>111</mml:m Physical Review B, 2010, 81, . | 1.1 | 11 |
| 138 | The layered ferromagnet Cs2AgF4: Antiferromagnetic inter-layer coupling driven by magnetic dipole-dipole interactions. Zeitschrift FÃ¼r Kristallographie, 2010, 225, . | 1.1 | 15 |
| 139 | Theoretical Investigation of the Magnetic Structure and Ferroelectric Polarization of the Multiferroic Langasite Ba<sub>3</sub>NbFe<sub>3</sub>Si<sub>2</sub>O<sub>14</sub>. Chemistry of Materials, 2010, 22, 5290-5295. | 3.2 | 26 |
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