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List of Publications by Year in Descending Order

157 papers	6,335 citations	38 h-index	75 g-index
165 ext. papers	7,301 ext. citations	5.8 avg, IF	5.99 L-index

#	Paper	IF	Citations
157	Room-Temperature Ferroelectricity in 1T^{0}-ReS_{2} Multilayers.. *Physical Review Letters*, **2022**, 128, 067601	7.4	5
156	Enabling High Loading in Single-Atom Catalysts on Bare Substrate with Chemical Scissors by Saturating the Anchoring Sites.. *Small*, **2022**, e2200073	11	3
155	Enabling High Loading in Single-Atom Catalysts on Bare Substrate with Chemical Scissors by Saturating the Anchoring Sites (Small 19/2022). *Small*, **2022**, 18, 2270098	11	1
154	Built-in electric field control of magnetic coupling in van der Waals semiconductors. *Physical Review B*, **2021**, 103,	3.3	4
153	Modulation on the Iron Centers by Selective Synthesis of Organic Ligands with Stereo-Specific Conformations. *Small*, **2021**, 17, e2008036	11	
152	Controllable vdW Contacts between the Ferroelectric In2Se3 Monolayer and Two-Dimensional Metals. *Journal of Physical Chemistry C*, **2021**, 125, 10738-10746	3.8	5
151	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	3.8	2
150	Trimetallic Octahedral NiCoW Phosphoxide Sprouted from Plasma-Defect-Engineered NiCo Support for Ultrahigh-Performance Electrocatalytic Hydrogen Evolution. *ACS Sustainable Chemistry and Engineering*, **2021**, 9, 7454-7465	8.3	7
149	Nature of spin-lattice coupling in two-dimensional CrI3 and CrGeTe3. *Science China: Physics, Mechanics and Astronomy*, **2021**, 64, 1	3.6	2
148	Graphene-mediated ferromagnetic coupling in the nickel nano-islands/graphene hybrid. *Science Advances*, **2021**, 7,	14.3	2
147	Substitutionally Dispersed High-Oxidation CoOx Clusters in the Lattice of Rutile TiO2 Triggering Efficient Co?Ti Cooperative Catalytic Centers for Oxygen Evolution Reactions. *Advanced Functional Materials*, **2021**, 31, 2009610	15.6	38
146	Selective Construction of Magic Hierarchical MetalOrganic Clusters on Surfaces. *Journal of Physical Chemistry C*, **2021**, 125, 358-365	3.8	3
145	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	3	
144	Two-dimensional metal-free boron chalcogenides BX (X = Se and Te) as photocatalysts for water splitting under visible light. *Nanoscale*, **2021**, 13, 3627-3632	7.7	2
143	Dimension effect on ferroelectricity: a first-principles study on GeS nanoribbons. *Physical Chemistry Chemical Physics*, **2021**, 23, 18863-18868	3.6	1
142	Improved contact properties of graphene-metal hybrid interfaces by grain boundaries. *Applied Surface Science*, **2021**, 563, 150392	6.7	
141	Manipulating the Raman scattering rotation magnetic field in an MoS monolayer.. *RSC Advances*, **2021**, 11, 4035-4041	3.7	0

140	Unconventional distortion induced two-dimensional multiferroicity in a CrO monolayer. *Nanoscale*, **2021**, 13, 13048-13056	7.7	1
139	Giant Biquadratic Exchange in 2D Magnets and Its Role in Stabilizing Ferromagnetism of NiCl_{2} Monolayers.. *Physical Review Letters*, **2021**, 127, 247204	7.4	1
138	Prediction of room-temperature ferromagnetism in a two-dimensional direct band gap semiconductor. *Nanoscale*, **2020**, 12, 15670-15676	7.7	12
137	Electrical Control of Magnetic Phase Transition in a Type-I Multiferroic Double-Metal Trihalide Monolayer. *Physical Review Letters*, **2020**, 124, 067602	7.4	38
136	Switchable encapsulation of polysulfides in the transition between sulfur and lithium sulfide. *Nature Communications*, **2020**, 11, 845	17.4	51
135	Discovery of twin orbital-order phases in ferromagnetic semiconducting VI monolayer. *Physical Chemistry Chemical Physics*, **2020**, 22, 512-517	3.6	18
134	Tunable ferroelectric single-atom catalysis of CO oxidation using a Pt/In2Se3 monolayer. *Journal of Materials Chemistry A*, **2020**, 8, 20725-20731	13	7
133	Water-sprouted, plasma-enhanced Ni-Co phospho-nitride nanosheets boost electrocatalytic hydrogen and oxygen evolution. *Chemical Engineering Journal*, **2020**, 402, 126257	14.7	26
132	Tuning Electronic and Magnetic Properties of Two-Dimensional Ferromagnetic Semiconductor CrI3 through Adsorption of Benzene. *Journal of Physical Chemistry C*, **2020**, 124, 22143-22149	3.8	10
131	Surface-sensitive magnetic characterization technique for ultrathin ferromagnetic film with perpendicular magnetic anisotropy. *AIP Advances*, **2020**, 10, 065019	1.5	
130	The Janus structures of group-III chalcogenide monolayers as promising photocatalysts for water splitting. *Applied Surface Science*, **2019**, 478, 522-531	6.7	40
129	Quinone-Facilitated Coordinated Bipyrene and Polypyrene on Au(111) by Capture of Gold Adatoms. *Journal of Physical Chemistry C*, **2019**, 123, 16281-16287	3.8	6
128	High-Temperature Ferromagnetism in an FeP Monolayer with a Large Magnetic Anisotropy. *Journal of Physical Chemistry Letters*, **2019**, 10, 2733-2738	6.4	50
127	Computational Dissection of 2D SiC7 Monolayer: A Direct Band Gap Semiconductor and High Power Conversion Efficiency. *Advanced Theory and Simulations*, **2019**, 2, 1900058	3.5	8
126	Room-temperature magnetism and tunable energy gaps in edge-passivated zigzag graphene quantum dots. *Npj 2D Materials and Applications*, **2019**, 3,	8.8	19
125	Mechanical, Electronic, and Magnetic Properties of NiX (X = Cl, Br, I) Layers. *ACS Omega*, **2019**, 4, 5714-5721	3.7	20
124	First-Principles Prediction of Room-Temperature Ferromagnetic Semiconductor MnS2 via Isovalent Alloying. *Journal of Physical Chemistry C*, **2019**, 123, 10114-10119	3.8	19
123	Giant Band Gap Reduction and Insulator−Metal Transition in Two-Dimensional InX (X = Cl, Br, I) Layers. *Journal of Physical Chemistry C*, **2019**, 123, 21763-21767	3.8	3

122	Hydrogen Induced Etching Features of Wrinkled Graphene Domains. *Nanomaterials*, **2019**, 9,	5.4	2
121	Substrate-induced half-metallic property in epitaxial silicene. *Europhysics Letters*, **2019**, 126, 57006	1.6	1
120	Ultra-High-Temperature Ferromagnetism in Intrinsic Tetrahedral Semiconductors. *Journal of the American Chemical Society*, **2019**, 141, 12413-12418	16.4	20
119	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	6.7	9
118	Boosting the Curie Temperature of Two-Dimensional Semiconducting CrI3 Monolayer through van der Waals Heterostructures. *Journal of Physical Chemistry C*, **2019**, 123, 17987-17993	3.8	38
117	Accurate K-edge X-ray photoelectron and absorption spectra of g-CN nanosheets by first-principles simulations and reinterpretations. *Physical Chemistry Chemical Physics*, **2019**, 21, 22819-22830	3.6	29
116	Progress and prospects in low-dimensional multiferroic materials. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1409	7.9	30
115	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	3	1
114	Effect of Coulomb Correlation on the Magnetic Properties of Mn Clusters. *Journal of Physical Chemistry A*, **2018**, 122, 4350-4356	2.8	4
113	Ultrathin molybdenum disulfide/carbon nitride nanosheets with abundant active sites for enhanced hydrogen evolution. *Nanoscale*, **2018**, 10, 1766-1773	7.7	46
112	Designing half-metallic ferromagnetism by a new strategy: an example of superhalogen modified graphitic C3N4. *Journal of Materials Chemistry C*, **2018**, 6, 1709-1714	7.1	14
111	Prediction of Intrinsic Ferromagnetic Ferroelectricity in a Transition-Metal Halide Monolayer. *Physical Review Letters*, **2018**, 120, 147601	7.4	149
110	Atomically thin mononitrides SiN and GeN: New two-dimensional wide band gap semiconductors. *Europhysics Letters*, **2018**, 122, 47002	1.6	3
109	Synthesis of Amorphous Carbon Film in Ethanol Inverse Diffusion Flames. *Nanomaterials*, **2018**, 8,	5.4	1
108	Toward Intrinsic Room-Temperature Ferromagnetism in Two-Dimensional Semiconductors. *Journal of the American Chemical Society*, **2018**, 140, 11519-11525	16.4	170
107	Atomically dispersed tungsten on metal halide monolayer as a ferromagnetic Chern insulator. *Physical Review B*, **2018**, 98,	3.3	5
106	Efficient Carrier Separation and Band Structure Tuning of Two-Dimensional C2N/GaTe van der Waals Heterostructure. *Journal of Physical Chemistry C*, **2018**, 122, 15892-15902	3.8	32
105	Hexagonal Boron Nitride–Metal Junction: Removing the Schottky Barriers by Grain Boundary. *Advanced Theory and Simulations*, **2018**, 1, 1800045	3.5	4

104	Band gap engineering and visible light response for GaS monolayer by isovalent anion-cation codoping. *Materials Chemistry and Physics*, **2017**, 198, 275-282	4.4	13
103	Van der Waals bilayer antimonene: A promising thermophotovoltaic cell material with 31% energy conversion efficiency. *Nano Energy*, **2017**, 38, 561-568	17.1	78
102	Stabilization of the Metastable Lead Iodide Perovskite Phase via Surface Functionalization. *Nano Letters*, **2017**, 17, 4405-4414	11.5	151
101	Quantum anomalous Hall effect in ferromagnetic transition metal halides. *Physical Review B*, **2017**, 95,	3.3	69
100	Edge-Modified Graphene Nanoribbons: Appearance of Robust Spiral Magnetism. *Journal of Physical Chemistry C*, **2017**, 121, 1371-1376	3.8	11
99	Prediction of another semimetallic silicene allotrope with Dirac fermions. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2017**, 381, 3754-3759	2.3	22
98	A promising two-dimensional channel material: monolayer antimonide phosphorus. *Science China Materials*, **2016**, 59, 648-656	7.1	22
97	High-capacity hydrogen storage in Li-adsorbed g-C3N4. *Materials Chemistry and Physics*, **2016**, 180, 440-444	4.4	12
96	Realizing half-metallicity in K2CoF4 exfoliated nanosheets via defect engineering. *Physical Chemistry Chemical Physics*, **2016**, 18, 15765-73	3.6	3
95	Superhalogens as building blocks of two-dimensional organic-inorganic hybrid perovskites for optoelectronics applications. *Nanoscale*, **2016**, 8, 17836-17842	7.7	32
94	Cobalt Sulfide/Graphene Composite Hydrogel as Electrode for High-Performance Pseudocapacitors. *Scientific Reports*, **2016**, 6, 21717	4.9	91
93	New Ferroelectric Phase in Atomic-Thick Phosphorene Nanoribbons: Existence of in-Plane Electric Polarization. *Nano Letters*, **2016**, 16, 8015-8020	11.5	46
92	Electride: from computational characterization to theoretical design. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2016**, 6, 430-440	7.9	31
91	Semiconducting Group 15 Monolayers: A Broad Range of Band Gaps and High Carrier Mobilities. *Angewandte Chemie - International Edition*, **2016**, 55, 1666-9	16.4	535
90	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	3.7	3
89	Semiconducting Group 15 Monolayers: A Broad Range of Band Gaps and High Carrier Mobilities. *Angewandte Chemie*, **2016**, 128, 1698-1701	3.6	254
88	Half-metallicity obtained in silicene nanosheet by nitrogenation engineering. *Journal of Applied Physics*, **2016**, 120, 234303	2.5	9
87	Quantum Phase Transition in Germanene and Stanene Bilayer: From Normal Metal to Topological Insulator. *Journal of Physical Chemistry Letters*, **2016**, 7, 1919-24	6.4	26

86	Valley contrasting in epitaxial growth of In/Tl homoatomic monolayer with anomalous Nernst conductance. *Physical Review B*, **2016**, 94,	3.3	5
85	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	2.3	3
84	Theoretical Prediction of Phosphorene and Nanoribbons As Fast-Charging Li Ion Battery Anode Materials. *Journal of Physical Chemistry C*, **2015**, 119, 6923-6928	3.8	83
83	Theoretical understanding of magnetic and electronic structures of Ti3C2 monolayer and its derivatives. *Solid State Communications*, **2015**, 222, 9-13	1.6	28
82	A promising way to open an energy gap in bilayer graphene. *Nanoscale*, **2015**, 7, 17096-101	7.7	9
81	Vacancy-induced insulator □direct spin gapless semiconductor □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	2.3	7
80	Atomically Thin Transition-Metal Dinitrides: High-Temperature Ferromagnetism and Half-Metallicity. *Nano Letters*, **2015**, 15, 8277-81	11.5	132
79	A theoretical study on the structural and physical properties of the ground-state CaC. *Solid State Communications*, **2015**, 203, 10-15	1.6	2
78	Coexistence of metallic and insulating-like states in graphene. *Scientific Reports*, **2015**, 5, 8974	4.9	3
77	Two-dimensional silicon monolayers generated on c-BN(111) substrate. *Physical Chemistry Chemical Physics*, **2015**, 17, 15694-700	3.6	9
76	Magnetic and electronic properties of frustrated spin dimer compound K2Fe2B2O7: A first-principles calculation. *Solid State Communications*, **2015**, 220, 77-80	1.6	
75	Electronic and magnetic properties of an AlN monolayer doped with first-row elements: a first-principles study. *RSC Advances*, **2015**, 5, 18352-18358	3.7	37
74	MnO2 nanorods intercalating graphene oxide/polyaniline ternary composites for robust high-performance supercapacitors. *Scientific Reports*, **2014**, 4, 4824	4.9	176
73	Will a graphitic-like ZnO single-layer be an ideal substrate for graphene?. *RSC Advances*, **2014**, 4, 17478	3.7	13
72	A B-C-N hybrid porous sheet: an efficient metal-free visible-light absorption material. *Physical Chemistry Chemical Physics*, **2014**, 16, 4299-304	3.6	11
71	A promising monolayer membrane for oxygen separation from harmful gases: nitrogen-substituted polyphenylene. *Nanoscale*, **2014**, 6, 9960-4	7.7	47
70	Ferroelectric-like structural transition in metallic LiOsO3. *RSC Advances*, **2014**, 4, 26843	3.7	6
69	Sandwich-structured MnO2/polypyrrole/reduced graphene oxide hybrid composites for high-performance supercapacitors. *RSC Advances*, **2014**, 4, 9898-9904	3.7	101

68	Improved permeability and selectivity in porous graphene for hydrogen purification. *Physical Chemistry Chemical Physics*, **2014**, 16, 25755-9	3.6	35
67	Electronic properties and hydrogen storage application of designed porous nanotubes from a polyphenylene network. *International Journal of Hydrogen Energy*, **2014**, 39, 18966-18975	6.7	28
66	Theoretical study of CO oxidation on cationic, neutral, and anionic AuM dimers (M = Pd and Ag). *Journal of Molecular Modeling*, **2014**, 20, 2313	2	4
65	The effect of oxygen vacancy on the half-metallic nature of double perovskite Sr2FeMoO6: A theoretical study. *Solid State Communications*, **2014**, 177, 57-60	1.6	20
64	Xiang et al. reply. *Physical Review Letters*, **2014**, 112, 199802	7.4	2
63	The effect of biaxial mechanical strain on the physical properties of double perovskite Sr2FeMoO6: A theoretical study. *Solid State Communications*, **2014**, 191, 70-75	1.6	16
62	Tunable band gap and hydrogen adsorption property of a two-dimensional porous polymer by nitrogen substitution. *Physical Chemistry Chemical Physics*, **2013**, 15, 666-70	3.6	20
61	High-temperature ferro-electricity in two-dimensional atomic crystal. *Applied Physics Letters*, **2013**, 103, 193103	3.4	26
60	Stability of graphitic-like zinc oxide layers under carriers doping: a first-principles study. *Nanoscale*, **2013**, 5, 12111-4	7.7	9
59	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, 16120-6	3.6	78
58	The strain effect on colossal oxygen ionic conductivity in nanoscale zirconia electrolytes: a first-principles-based study. *Physical Chemistry Chemical Physics*, **2013**, 15, 2692-7	3.6	16
57	Two-Dimensional Hexagonal Transition-Metal Oxide for Spintronics. *Journal of Physical Chemistry Letters*, **2013**, 4, 1120-5	6.4	49
56	d0 magnetism in semiconductors through confining delocalized atomic orbitals. *Applied Physics Letters*, **2013**, 102, 022422	3.4	9
55	Towards direct-gap silicon phases by the inverse band structure design approach. *Physical Review Letters*, **2013**, 110, 118702	7.4	112
54	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	6.7	33
53	Geometric and Electronic Structures as well as Thermodynamic Stability of Hexyl-Modified Silicon Nanosheet. *Journal of Physical Chemistry C*, **2013**, 117, 13283-13288	3.8	15
52	Influences of lithium doping and fullerene impregnation on hydrogen storage in metal organic frameworks. *Molecular Simulation*, **2013**, 39, 968-974	2	10
51	Stabilizing intrinsic defects in SnO2. *Physical Review B*, **2013**, 87,	3.3	38

50	Carrier-tunable magnetism of graphene with single-atom vacancy. *Journal of Applied Physics*, **2013**, 113, 213709	2.5	7
49	Biaxial strain effect on the electronic and magnetic phase transitions in double perovskite La2FeMnO6: A first-principles study. *Journal of Applied Physics*, **2013**, 114, 063713	2.5	14
48	Two-dimensional organometallic porous sheets with possible high-temperature ferromagnetism. *Nanoscale*, **2012**, 4, 5304-7	7.7	22
47	Visible-Light-Absorption in Graphitic C3N4 Bilayer: Enhanced by Interlayer Coupling. *Journal of Physical Chemistry Letters*, **2012**, 3, 3330-3334	6.4	123
46	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, 6890-7	5.1	16
45	Half-metallicity in organic single porous sheets. *Journal of the American Chemical Society*, **2012**, 134, 5718-21	8.4	87
44	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	3.8	68
43	Unzipping carbon nanotubes into nanoribbons upon oxidation: a first-principles study. *Nanoscale*, **2012**, 4, 1254-7	7.7	16
42	Why the Band Gap of Graphene Is Tunable on Hexagonal Boron Nitride. *Journal of Physical Chemistry C*, **2012**, 116, 3142-3146	3.8	88
41	. *Journal of Physical Chemistry C*, **2012**, 116, 11336-11342	3.8	150
40	First-principles investigations on the magnetic structure of □NaMnO□*Journal of Physics Condensed Matter*, **2012**, 24, 456002	1.8	4
39	Enhancing magnetic vacancies in semiconductors by strain. *Applied Physics Letters*, **2012**, 100, 072401	3.4	19
38	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, 7698-700	5.8	53
37	Density functional theory analysis of the interplay between Jahn-Teller instability, uniaxial magnetism, spin arrangement, metal-metal interaction, and spin-orbit coupling in Ca3CoMO6 (M = Co, Rh, Ir). *Inorganic Chemistry*, **2011**, 50, 1758-66	5.1	19
36	Density Functional Investigation of the Difference in the Magnetic Structures of the Layered Triangular Antiferromagnets CuFeO2 and AgCrO2. *Chemistry of Materials*, **2011**, 23, 4181-4185	9.6	6
35	Graphene Nanoribbons: Geometric, Electronic, and Magnetic Properties **2011**,		18
34	Density functional predictions of new silicon allotropes: Electronic properties and potential applications to Li-battery anode materials. *Solid State Communications*, **2011**, 151, 1228-1230	1.6	18
33	Site-selected doping in silicon nanowires by an external electric field. *Nanoscale*, **2011**, 3, 3620-2	7.7	3

32	Half-Metallic Dirac Point in B-Edge Hydrogenated BN Nanoribbons. *Journal of Physical Chemistry C*, **2011**, 115, 17252-17254	3.8	35
31	Single-ion anisotropy, Dzyaloshinskii-Moriya interaction, and negative magnetoresistance of the spin-12 pyrochlore R2V2O7. *Physical Review B*, **2011**, 83,	3.3	33
30	On the high magnetic-ordering temperature of the 5d magnetic oxide Ca3LiOsO6 crystallizing in a trigonal crystal structure: density functional analysis. *Inorganic Chemistry*, **2011**, 50, 4182-6	5.1	10
29	Predicting the spin-lattice order of frustrated systems from first principles. *Physical Review B*, **2011**, 84,	3.3	166
28	General theory for the ferroelectric polarization induced by spin-spiral order. *Physical Review Letters*, **2011**, 107, 157202	7.4	81
27	Ferrimagnetism in zigzag graphene nanoribbons induced by main-group adatoms. *Applied Physics Letters*, **2010**, 96, 102503	3.4	37
26	Electrical rectification by selective wave-function coupling in small Ag clusters on Si(111)(7 7). *Physical Review B*, **2010**, 81,	3.3	11
25	The layered ferromagnet Cs2AgF4: Antiferromagnetic inter-layer coupling driven by magnetic dipole-dipole interactions. *Zeitschrift F Kristallographie*, **2010**, 225,		13
24	Theoretical Investigation of the Magnetic Structure and Ferroelectric Polarization of the Multiferroic Langasite Ba3NbFe3Si2O14. *Chemistry of Materials*, **2010**, 22, 5290-5295	9.6	24
23	Orbital order and partial electronic delocalization in a triangular magnetic metal Ag2MnO2. *Physical Review B*, **2010**, 81,	3.3	23
22	Prediction for room-temperature half-metallic ferromagnetism in the half-fluorinated single layers of BN and ZnO. *Applied Physics Letters*, **2010**, 97, 122503	3.4	45
21	Pi-back-donation effect of the cyanide ligands on the electron correlation and charge transfer in Prussian blue RbMn[Fe(CN)(6)]. *Inorganic Chemistry*, **2010**, 49, 3086-8	5.1	17
20	On the importance of the interplaquette spin exchanges in Na3RuO4: density functional theory analysis of the spin exchange and magnetic properties. *Inorganic Chemistry*, **2010**, 49, 3025-8	5.1	11
19	Half-metallic ferromagnetism and large negative magnetoresistance in the new lacunar spinel GaTi3VS8. *Journal of the American Chemical Society*, **2010**, 132, 5704-10	16.4	46
18	Analysis of the magnetic structure and ferroelectric polarization of monoclinic MnSb(2)S(4) by density functional theory calculations. *Inorganic Chemistry*, **2010**, 49, 10956-9	5.1	10
17	Theoretical analysis of the spin exchange and magnetic dipole-dipole interactions leading to the magnetic structure of Ni3TeO6. *Inorganic Chemistry*, **2010**, 49, 7545-8	5.1	28
16	Thermodynamically stable single-side hydrogenated graphene. *Physical Review B*, **2010**, 82,	3.3	44
15	Ferroelectricity in Perovskites with s0 A-Site Cations: Toward Near-Room-Temperature Multiferroics. *Angewandte Chemie*, **2010**, 122, 1647-1650	3.6	8

14	Ferroelectricity in perovskites with s0 A-site cations: toward near-room-temperature multiferroics. *Angewandte Chemie - International Edition*, **2010**, 49, 1603-6	16.4	22
13	Origin of the Ising ferrimagnetism and spin-charge coupling in LuFe2O4. *Physical Review B*, **2009**, 80,	3.3	27
12	Magnetism of semiconductor-based magnetic tunnel junctions under electric field from first principles. *Applied Physics Letters*, **2009**, 94, 252102	3.4	2
11	Magnetic states of zigzag graphene nanoribbons from first principles. *Applied Physics Letters*, **2009**, 94, 223105	3.4	37
10	"Narrow" graphene nanoribbons made easier by partial hydrogenation. *Nano Letters*, **2009**, 9, 4025-30	11.5	115
9	Density-functional analysis of spin exchange and ferroelectric polarization in AgCrO2. *Physical Review B*, **2009**, 80,	3.3	25
8	Half-metallicity in edge-modified zigzag graphene nanoribbons. *Journal of the American Chemical Society*, **2008**, 130, 4224-5	16.4	587
7	Half-metallicity in hybrid BCN nanoribbons. *Journal of Chemical Physics*, **2008**, 129, 084712	3.9	129
6	MAGNETISM IN GRAPHENE SYSTEMS. *Nano*, **2008**, 03, 433-442	1.1	61
5	Will zigzag graphene nanoribbon turn to half metal under electric field?. *Applied Physics Letters*, **2007**, 91, 243116	3.4	285
4	Electronic structure of atomic Ti chains on semiconducting graphene nanoribbons: a first-principles study. *Journal of Chemical Physics*, **2007**, 127, 164706	3.9	30
3	First-principles study of interaction between H2 molecules and BN nanotubes with BN divacancies. *Journal of Chemical Physics*, **2007**, 127, 164718	3.9	18
2	Electron-induced ferromagnetic ordering of Co-doped ZnO. *Journal of Applied Physics*, **2007**, 102, 033915	2.5	39
1	First-principles calculations of the electronic and magnetic properties of Cs2AgF4. *Physical Review B*, **2007**, 76,	3.3	13