

# Wenhui Duan

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

389 papers	20,550 citations	69 h-index	131 g-index
410 ext. papers	23,635 ext. citations	6.1 avg, IF	6.94 L-index

#	Paper	IF	Citations
389	Realizing quinary charge states of solitary defects in two-dimensional intermetallic semiconductor.. <i>National Science Review</i> , <b>2022</b> , 9, nwab070	10.8	1
388	Chemical Potential Switching of the Anomalous Hall Effect in an Ultrathin Noncollinear Antiferromagnetic Metal.. <i>Advanced Materials</i> , <b>2022</b> , e2200487	24	1
387	Control of phase ordering and elastic properties in phase field crystals through three-point direct correlation.. <i>Physical Review E</i> , <b>2022</b> , 105, 044802	2.4	0
386	Interplay between quantum anomalous Hall effect and magnetic skyrmions.. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2022</b> , 119, e2122952119	11.5	0
385	Symmetry-adapted graph neural networks for constructing molecular dynamics force fields. <i>Science China: Physics, Mechanics and Astronomy</i> , <b>2021</b> , 64, 1	3.6	1
384	Anisotropic Full-Gap Superconductivity in 2M-WS Topological Metal with Intrinsic Proximity Effect. <i>Nano Letters</i> , <b>2021</b> , 21, 709-715	11.5	1
383	Large transport gap modulation in graphene via electric-field-controlled reversible hydrogenation. <i>Nature Electronics</i> , <b>2021</b> , 4, 254-260	28.4	7
382	What is the Role of Nb on Preferential Hydriding of Double-Phased Uranium, Stabilizing $\beta$ U, or Avoiding Hydrogen Aggregation?. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 9364-9370	3.8	
381	Accuracy trade-off between one-electron and excitonic spectra of cuprous halides in first-principles calculations. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 134704	3.9	0
380	Experimental Evidence of Chiral Symmetry Breaking in Kekulé-Ordered Graphene. <i>Physical Review Letters</i> , <b>2021</b> , 126, 206804	7.4	17
379	Boosting the Oxidative Potential of Polyethylene Glycol-Based Polymer Electrolyte to 4.36 V by Spatially Restricting Hydroxyl Groups for High-Voltage Flexible Lithium-Ion Battery Applications. <i>Advanced Science</i> , <b>2021</b> , 8, e2100736	13.6	11
378	High-Temperature Excitonic Bose-Einstein Condensate in Centrosymmetric Two-Dimensional Semiconductors. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 5479-5485	6.4	1
377	Ising Superconductivity and Its Hidden Variants. <i>Accounts of Materials Research</i> , <b>2021</b> , 2, 526-533	7.5	0
376	Growth of large scale PtTe, PtTe <sub>2</sub> and PtSe <sub>2</sub> films on a wide range of substrates. <i>Nano Research</i> , <b>2021</b> , 14, 1663-1667	10	11
375	Magnetic Moments Induced by Atomic Vacancies in Transition Metal Dichalcogenide Flakes. <i>Advanced Materials</i> , <b>2021</b> , 33, e2005465	24	18
374	Valley Depolarization Dynamics in Monolayer Transition-Metal Dichalcogenides: Role of the Satellite Valley. <i>Nano Letters</i> , <b>2021</b> , 21, 1785-1791	11.5	3
373	Light-Tunable Surface State and Hybridization Gap in Magnetic Topological Insulator MnBiTe. <i>Nano Letters</i> , <b>2021</b> , 21, 6080-6086	11.5	4

372	Lithium Storage Mechanism and Application of Micron-Sized Lattice-Reversible Binary Intermetallic Compounds as High-Performance Flexible Lithium-Ion Battery Anodes. <i>Small</i> , <b>2021</b> , e2105172	11	2
371	Nodal Flexible-surface Semimetals: Case of Carbon Nanotube Networks. <i>Nano Letters</i> , <b>2020</b> , 20, 5400-5407	7.5	15
370	Type-II Ising pairing in few-layer stanene. <i>Science</i> , <b>2020</b> , 367, 1454-1457	33.3	42
369	Excitons and Electron-Hole Liquid State in 2D Phase Group-IV Monochalcogenides. <i>Advanced Functional Materials</i> , <b>2020</b> , 30, 2000533	15.6	13
368	Hexagonal rare-earth manganites and ferrites: a review of improper ferroelectricity, magnetoelectric coupling, and unusual domain walls. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 14413-14432	3.6	15
367	Multi-ion Modulated Single-Step Synthesis of a Nanocarbon Embedded with a Defect-Rich Nanoparticle Catalyst for a High Loading Sulfur Cathode. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2020</b> , 12, 12727-12735	9.5	14
366	Single atomic cobalt catalyst significantly accelerates lithium ion diffusion in high mass loading Li <sub>2</sub> S cathode. <i>Energy Storage Materials</i> , <b>2020</b> , 28, 375-382	19.4	42
365	Spin-Triplet Excitonic Insulator: The Case of Semihydrogenated Graphene. <i>Physical Review Letters</i> , <b>2020</b> , 124, 166401	7.4	9
364	Berry curvature engineering by gating two-dimensional antiferromagnets. <i>Physical Review Research</i> , <b>2020</b> , 2,	3.9	12
363	Minimal phase-field crystal modeling of vapor-liquid-solid coexistence and transitions. <i>Physical Review Materials</i> , <b>2020</b> , 4,	3.2	2
362	Enhancement of superconductivity in organic-inorganic hybrid topological materials. <i>Science Bulletin</i> , <b>2020</b> , 65, 188-193	10.6	22
361	Topological semimetals from the perspective of first-principles calculations. <i>Journal of Applied Physics</i> , <b>2020</b> , 128, 191101	2.5	3
360	Tunable interlayer magnetism and band topology in van der Waals heterostructures of MnBi <sub>2</sub> Te <sub>4</sub> -family materials. <i>Physical Review B</i> , <b>2020</b> , 102,	3.3	13
359	Hidden physical effects in noncentrosymmetric crystals. <i>Physical Review B</i> , <b>2020</b> , 102,	3.3	3
358	High-Temperature Quantum Anomalous Hall Insulators in Lithium-Decorated Iron-Based Superconductor Materials. <i>Physical Review Letters</i> , <b>2020</b> , 125, 086401	7.4	11
357	Electronic States and Magnetic Response of MnBiTe by Scanning Tunneling Microscopy and Spectroscopy. <i>Nano Letters</i> , <b>2020</b> , 20, 3271-3277	11.5	34
356	First-principles calculation of optical responses based on nonorthogonal localized orbitals. <i>New Journal of Physics</i> , <b>2019</b> , 21, 093001	2.9	1
355	Magnetically controllable topological quantum phase transitions in the antiferromagnetic topological insulator MnBi <sub>2</sub> Te <sub>4</sub> . <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	45

354	Type-II Ising Superconductivity in Two-Dimensional Materials with Spin-Orbit Coupling. <i>Physical Review Letters</i> , <b>2019</b> , 123, 126402	7.4	30
353	Understanding the origin of bandgap problem in transition and post-transition metal oxides. <i>Journal of Chemical Physics</i> , <b>2019</b> , 151, 124703	3.9	3
352	Effective chemical potential for non-equilibrium systems and its application to molecular beam epitaxy of Bi <sub>2</sub> Se <sub>3</sub> . <i>Nanoscale Advances</i> , <b>2019</b> , 1, 470-475	5.1	6
351	Continuous, Ultra-lightweight, and Multipurpose Super-aligned Carbon Nanotube Tapes Viable over a Wide Range of Temperatures. <i>Nano Letters</i> , <b>2019</b> , 19, 6756-6764	11.5	9
350	Crossover from 2D metal to 3D Dirac semimetal in metallic PtTe <sub>2</sub> films with local Rashba effect. <i>Science Bulletin</i> , <b>2019</b> , 64, 1044-1048	10.6	29
349	Two-dimensional ferromagnetic-ferroelectric multiferroics in violation of the d <sub>0</sub> rule. <i>Physical Review B</i> , <b>2019</b> , 99,	3.3	34
348	Half-Excitonic Insulator: A Single-Spin Bose-Einstein Condensate. <i>Physical Review Letters</i> , <b>2019</b> , 122, 236402	7.4	10
347	Experimental Realization of an Intrinsic Magnetic Topological Insulator*. <i>Chinese Physics Letters</i> , <b>2019</b> , 36, 076801	1.8	260
346	Intrinsic magnetic topological insulators in van der Waals layered MnBiTe-family materials. <i>Science Advances</i> , <b>2019</b> , 5, eaaw5685	14.3	330
345	Density functional theory calculations: A powerful tool to simulate and design high-performance energy storage and conversion materials. <i>Progress in Natural Science: Materials International</i> , <b>2019</b> , 29, 247-255	3.6	37
344	High areal capacity flexible sulfur cathode based on multi-functionalized super-aligned carbon nanotubes. <i>Nano Research</i> , <b>2019</b> , 12, 1105-1113	10	25
343	Group VB transition metal dichalcogenides for oxygen reduction reaction and strain-enhanced activity governed by p-orbital electrons of chalcogen. <i>Nano Research</i> , <b>2019</b> , 12, 925-930	10	27
342	Prediction of Stoner-Type Magnetism in Low-Dimensional Electrides. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 5003-5009	3.8	12
341	Dimensional Crossover and Topological Phase Transition in Dirac Semimetal NaBi Films. <i>ACS Nano</i> , <b>2019</b> , 13, 9647-9654	16.7	17
340	Landau quantization of nearly degenerate bands and full symmetry classification of Landau level crossings. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	5
339	Coexistence of Superconductivity with Enhanced Charge Density Wave Order in the Two-Dimensional Limit of TaSe. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 4076-4081	6.4	20
338	Electronic structure of molecular beam epitaxy grown $\text{Te}^{\text{prime}}$ -MoTe <sub>2</sub> film and strain effect. <i>Chinese Physics B</i> , <b>2019</b> , 28, 107307	1.2	5
337	Anomalous Dirac Plasmons in 1D Topological Electrides. <i>Physical Review Letters</i> , <b>2019</b> , 123, 206402	7.4	14

336	Magnetic anisotropy of the two-dimensional ferromagnetic insulator MnBi <sub>2</sub> Te <sub>4</sub> . <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	24
335	Visualization of Dopant Oxygen Atoms in a Bi <sub>2</sub> Sr <sub>2</sub> CaCu <sub>2</sub> O <sub>8-x</sub> Superconductor. <i>Advanced Functional Materials</i> , <b>2019</b> , 29, 1903843	15.6	13
334	Rashba splitting in bilayer transition metal dichalcogenides controlled by electronic ferroelectricity. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	13
333	Ion intercalation engineering of electronic properties of two-dimensional crystals of 2H-TaSe <sub>2</sub> . <i>Physical Review Materials</i> , <b>2019</b> , 3,	3.2	4
332	Three-Dimensional Topological States of Phonons with Tunable Pseudospin Physics. <i>Research</i> , <b>2019</b> , 2019, 5173580	7.8	9
331	Manipulate the Electronic and Magnetic States in NiCo O Films through Electric-Field-Induced Protonation at Elevated Temperature. <i>Advanced Materials</i> , <b>2019</b> , 31, e1900458	24	39
330	Intrinsic Half-Metallicity in 2D Ternary Chalcogenides with High Critical Temperature and Controllable Magnetization Direction. <i>Advanced Functional Materials</i> , <b>2019</b> , 29, 1808380	15.6	34
329	Single anisotropic gap superconductivity and proximity effect in PbTaSe <sub>2</sub> . <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	6
328	Evidence of charge density wave with anisotropic gap in a monolayer VTe <sub>2</sub> film. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	25
327	Hidden metal-insulator transition in manganites synthesized via a controllable oxidation. <i>Science China Materials</i> , <b>2019</b> , 62, 577-585	7.1	6
326	Single-atom catalyst boosts electrochemical conversion reactions in batteries. <i>Energy Storage Materials</i> , <b>2019</b> , 18, 246-252	19.4	121
325	Pressure-induced Lifshitz transition in the type II Dirac semimetal PtTe <sub>2</sub> . <i>Science China: Physics, Mechanics and Astronomy</i> , <b>2019</b> , 62, 1	3.6	8
324	Elastic Properties and Fracture Behaviors of Biaxially Deformed, Polymorphic MoTe. <i>Nano Letters</i> , <b>2019</b> , 19, 761-769	11.5	31
323	Enhanced performance of lithium-sulfur batteries with an ultrathin and lightweight MoS <sub>2</sub> /carbon nanotube interlayer. <i>Journal of Power Sources</i> , <b>2018</b> , 389, 169-177	8.9	85
322	Unveiling Charge-Density Wave, Superconductivity, and Their Competitive Nature in Two-Dimensional NbSe. <i>Nano Letters</i> , <b>2018</b> , 18, 2924-2929	11.5	56
321	Revealing the Topology of Fermi-Surface Wave Functions from Magnetic Quantum Oscillations. <i>Physical Review X</i> , <b>2018</b> , 8,	9.1	20
320	Multifunctional Interlayer Based on Molybdenum Diphosphide Catalyst and Carbon Nanotube Film for Lithium-Sulfur Batteries. <i>Small</i> , <b>2018</b> , 14, 1702853	11	108
319	First-principles studies of the local structure and relaxor behavior of Pb(Mg <sub>1/3</sub> Nb <sub>2/3</sub> )O <sub>3</sub> PbTiO <sub>3</sub> -derived ferroelectric perovskite solid solutions. <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	14

318	Growth of atomically thick transition metal sulfide films on graphene/6H-SiC(0001) by molecular beam epitaxy. <i>Nano Research</i> , <b>2018</b> , 11, 4722-4727	10	32
317	Universal Descriptor for Large-Scale Screening of High-Performance MXene-Based Materials for Energy Storage and Conversion. <i>Chemistry of Materials</i> , <b>2018</b> , 30, 2687-2693	9.6	47
316	Berry phase and topological effects of phonons. <i>National Science Review</i> , <b>2018</b> , 5, 314-316	10.8	26
315	Resolving Deep Quantum-Well States in Atomically Thin 2H-MoTe Flakes by Nanoscale Angle-Resolved Photoemission Spectroscopy. <i>Nano Letters</i> , <b>2018</b> , 18, 4664-4668	11.5	7
314	Thermal Engineering in Low-Dimensional Quantum Devices: A Tutorial Review of Nonequilibrium Green's Function Methods. <i>Small Methods</i> , <b>2018</b> , 2, 1700343	12.8	12
313	Roles of Oxygen Vacancy in Improper Ferroelectrics. <i>Microscopy and Microanalysis</i> , <b>2018</b> , 24, 74-75	0.5	
312	Surface symmetry breaking and disorder effects on superconductivity in perovskite BaBi <sub>3</sub> epitaxial films. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	1
311	Realizing an intrinsic excitonic insulator by decoupling exciton binding energy from the minimum band gap. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	12
310	Widely tunable band gap in a multivalley semiconductor SnSe by potassium doping. <i>Physical Review Materials</i> , <b>2018</b> , 2,	3.2	12
309	Two-dimensional superconductivity and topological states in PdTe <sub>2</sub> thin films. <i>Physical Review Materials</i> , <b>2018</b> , 2,	3.2	36
308	Spin-Polarized Semiconducting Band Structure of Monolayer Graphene on Ni(111). <i>Physical Review Applied</i> , <b>2018</b> , 10,	4.3	4
307	Pseudo Dirac nodal sphere semimetal. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	20
306	Electrically tunable valleytronics in quantum anomalous Hall insulating transition metal trihalides. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	13
305	Evidence for a Quasi-One-Dimensional Charge Density Wave in CuTe by Angle-Resolved Photoemission Spectroscopy. <i>Physical Review Letters</i> , <b>2018</b> , 121, 206402	7.4	16
304	Saddle-Point Excitons and Their Extraordinary Light Absorption in 2D D <sub>3h</sub> Phase Group-IV Monochalcogenides. <i>Advanced Functional Materials</i> , <b>2018</b> , 28, 1804581	15.6	18
303	Modulating the Electronic Properties of Graphene by Self-Organized Sulfur Identical Nanoclusters and Atomic Superlattices Confined at an Interface. <i>ACS Nano</i> , <b>2018</b> , 12, 10984-10991	16.7	14
302	Epitaxial growth of ultraflat stanene with topological band inversion. <i>Nature Materials</i> , <b>2018</b> , 17, 1081-1086	10.8	175
301	Binary Two-Dimensional Honeycomb Lattice with Strong Spin-Orbit Coupling and Electron-Hole Asymmetry. <i>Physical Review Letters</i> , <b>2018</b> , 121, 126801	7.4	27

300	Interface reconstruction with emerging charge ordering in hexagonal manganite. <i>Science Advances</i> , <b>2018</b> , 4, eaar4298	14.3	28
299	Effect of Hartree-Fock pseudopotentials on local density functional theory calculations. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 18844-18849	3.6	4
298	General criterion to distinguish between Schottky and Ohmic contacts at the metal/two-dimensional semiconductor interface. <i>Nanoscale</i> , <b>2017</b> , 9, 2068-2073	7.7	26
297	Tunable Structural, Electronic, and Optical Properties of Layered Two-Dimensional C <sub>2</sub> N and MoS <sub>2</sub> van der Waals Heterostructure as Photovoltaic Material. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 36543-3660	3.8	166
296	Liquid-Phase Electrochemical Scanning Electron Microscopy for In Situ Investigation of Lithium Dendrite Growth and Dissolution. <i>Advanced Materials</i> , <b>2017</b> , 29, 1606187	24	91
295	Direct observation of spin-layer locking by local Rashba effect in monolayer semiconducting PtSe film. <i>Nature Communications</i> , <b>2017</b> , 8, 14216	17.4	110
294	Phonon-mediated high-T superconductivity in hole-doped diamond-like crystalline hydrocarbon. <i>Scientific Reports</i> , <b>2017</b> , 7, 1464	4.9	4
293	Lithium Dendrites: Liquid-Phase Electrochemical Scanning Electron Microscopy for In Situ Investigation of Lithium Dendrite Growth and Dissolution (Adv. Mater. 13/2017). <i>Advanced Materials</i> , <b>2017</b> , 29,	24	1
292	Emerging topological states in quasi-two-dimensional materials. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2017</b> , 7, e1296	7.9	17
291	Pressure-Induced Multiferroics via Pseudo Jahn-Teller Effects and Novel Couplings. <i>Advanced Functional Materials</i> , <b>2017</b> , 27, 1604513	15.6	22
290	Carbon-Nanotube-Confined Vertical Heterostructures with Asymmetric Contacts. <i>Advanced Materials</i> , <b>2017</b> , 29, 1702942	24	14
289	Experimental evidence for type-II Dirac semimetal in PtSe <sub>2</sub> . <i>Physical Review B</i> , <b>2017</b> , 96,	3.3	142
288	Low-energy transmission electron diffraction and imaging of large-area graphene. <i>Science Advances</i> , <b>2017</b> , 3, e1603231	14.3	18
287	High quality atomically thin PtSe <sub>2</sub> films grown by molecular beam epitaxy. <i>2D Materials</i> , <b>2017</b> , 4, 045015	5.9	113
286	Dirac semimetal phase in hexagonal LiZnBi. <i>Physical Review B</i> , <b>2017</b> , 96,	3.3	19
285	First-principles calculation of nonlinear optical responses by Wannier interpolation. <i>Physical Review B</i> , <b>2017</b> , 96,	3.3	29
284	Lorentz-violating type-II Dirac fermions in transition metal dichalcogenide PtTe. <i>Nature Communications</i> , <b>2017</b> , 8, 257	17.4	239
283	Finite-size effects and spin texture of hourglass fermions in KHgSb films. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	1

282	Atomic Mechanism of Hybridization-Dependent Surface Reconstruction with Tailored Functionality in Hexagonal Multiferroics. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2017</b> , 9, 27322-27331	9.5	10
281	Voltage-controllable colossal magnetocrystalline anisotropy in single-layer transition metal dichalcogenides. <i>Physical Review B</i> , <b>2017</b> , 96,	3.3	31
280	Model for topological phononics and phonon diode. <i>Physical Review B</i> , <b>2017</b> , 96,	3.3	63
279	Structural and electronic phase transitions in ferromagnetic monolayer VS <sub>2</sub> induced by charge doping. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	36
278	Scaling Universality between Band Gap and Exciton Binding Energy of Two-Dimensional Semiconductors. <i>Physical Review Letters</i> , <b>2017</b> , 118, 266401	7.4	107
277	First-principles study of Na-intercalated bilayer NbSe <sub>2</sub> : Suppressed charge-density wave and strain-enhanced superconductivity. <i>Physical Review B</i> , <b>2017</b> , 96,	3.3	22
276	Giant enhancement of the intrinsic spin Hall conductivity in Hg <sub>1-x</sub> Te via substitutional doping. <i>Physical Review B</i> , <b>2017</b> , 96,	3.3	38
275	Pseudospins and Topological Effects of Phonons in a Kekulé Lattice. <i>Physical Review Letters</i> , <b>2017</b> , 119, 255901	7.4	53
274	Electronic and crystal structure changes induced by in-plane oxygen vacancies in multiferroic YMnO <sub>3</sub> . <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	24
273	Stability investigations on the non-vdW-exfoliated surfaces of the topological insulator Bi <sub>2</sub> Te <sub>3</sub> : A first-principles study. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	5
272	Topological nodal-line semimetals in alkaline-earth stannides, germanides, and silicides. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	160
271	Stable Dirac semimetal in the allotropes of group-IV elements. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	11
270	Discovery of robust in-plane ferroelectricity in atomic-thick SnTe. <i>Science</i> , <b>2016</b> , 353, 274-8	33.3	470
269	Energy gaps of atomically precise armchair graphene sidewall nanoribbons. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	38
268	Electronic properties of SnTe-class topological crystalline insulator materials. <i>Chinese Physics B</i> , <b>2016</b> , 25, 117313	1.2	9
267	Heavy Dirac fermions in a graphene/topological insulator hetero-junction. <i>2D Materials</i> , <b>2016</b> , 3, 034006	5.9	11
266	Manipulation of Magnetic Properties by Oxygen Vacancies in Multiferroic YMnO <sub>3</sub> . <i>Advanced Functional Materials</i> , <b>2016</b> , 26, 3589-3598	15.6	40
265	Plasmons of topological crystalline insulator SnTe with nanostructured patterns. <i>RSC Advances</i> , <b>2016</b> , 6, 56042-56047	3.7	1

264	Defect energetics and magnetic properties of 3d-transition-metal-doped topological crystalline insulator SnTe. <i>Science China: Physics, Mechanics and Astronomy</i> , <b>2016</b> , 59, 1	3.6	3
263	Tuning thermoelectricity in a Bi <sub>2</sub> Se <sub>3</sub> topological insulator via varied film thickness. <i>New Journal of Physics</i> , <b>2016</b> , 18, 015008	2.9	33
262	Topological insulators: Quasi-1D topological insulators. <i>Nature Materials</i> , <b>2016</b> , 15, 129-30	27	6
261	A few-layered Ti <sub>3</sub> C <sub>2</sub> nanosheet/glass fiber composite separator as a lithium polysulphide reservoir for high-performance lithium-sulfur batteries. <i>Journal of Materials Chemistry A</i> , <b>2016</b> , 4, 5993-5998	13	112
260	Large negative thermal expansion in non-perovskite lead-free ferroelectric Sn <sub>2</sub> P <sub>2</sub> S <sub>6</sub> . <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 6247-51	3.6	19
259	Pressure and strain effects of hexagonal rare-earth manganites: a first-principles study. <i>Journal of Physics Condensed Matter</i> , <b>2016</b> , 28, 126002	1.8	14
258	Prediction of silicon-based room temperature quantum spin Hall insulator via orbital mixing. <i>Europhysics Letters</i> , <b>2016</b> , 113, 67003	1.6	5
257	Wide-band-gap wrinkled nanoribbon-like structures in a continuous metallic graphene sheet. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	4
256	First-principles study of line-defect-embedded zigzag graphene nanoribbons: electronic and magnetic properties. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 12350-6	3.6	19
255	Deterministic Role of Concentration Surplus of Cation Vacancy over Anion Vacancy in Bipolar Memristive NiO. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2016</b> , 8, 11583-91	9.5	18
254	Experimental observation of topological Fermi arcs in type-II Weyl semimetal MoTe <sub>2</sub> . <i>Nature Physics</i> , <b>2016</b> , 12, 1105-1110	16.2	506
253	Type-II Dirac fermions in the PtSe <sub>2</sub> class of transition metal dichalcogenides. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	187
252	Scanning Tunneling Microscopy of the Magnetism of a Single Carbon Vacancy in Graphene. <i>Physical Review Letters</i> , <b>2016</b> , 117, 166801	7.4	87
251	Prediction of a stable post-post-perovskite structure from first principles. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	20
250	Robust gapless surface state and Rashba-splitting bands upon surface deposition of magnetic Cr on Bi <sub>2</sub> Se <sub>3</sub> . <i>Nano Letters</i> , <b>2015</b> , 15, 2031-6	11.5	27
249	Electronic analog of chiral metamaterial: Helicity-resolved filtering and focusing of Dirac fermions in thin films of topological materials. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	7
248	Ultra-stable small diameter hybrid transition metal dichalcogenide nanotubes X-M-Y (X, Y = S, Se, Te; M = Mo, W, Nb, Ta): a computational study. <i>Nanoscale</i> , <b>2015</b> , 7, 13586-90	7.7	31
247	First principles study of ruthenium(II) sensitizer adsorption on anatase TiO <sub>2</sub> (001) surface. <i>RSC Advances</i> , <b>2015</b> , 5, 60230-60236	3.7	6

246	Tunable Magnetism in Transition-Metal-Decorated Phosphorene. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 10059-10063	3.8	96
245	Structural phase transition and electronic structure evolution in Ir 1 $\times$ Pt x Te 2 studied by scanning tunneling microscopy. <i>Science Bulletin</i> , <b>2015</b> , 60, 798-805	10.6	10
244	Enhanced thermoelectric figure of merit in thin GaAs nanowires. <i>Nanoscale</i> , <b>2015</b> , 7, 8776-81	7.7	21
243	Molecular Beam Epitaxy-Grown SnSe in the Rock-Salt Structure: An Artificial Topological Crystalline Insulator Material. <i>Advanced Materials</i> , <b>2015</b> , 27, 4150-4	24	64
242	Electrically tunable multiple Dirac cones in thin films of the (LaO) <sub>2</sub> (SbSe <sub>2</sub> ) <sub>2</sub> family of materials. <i>Nature Communications</i> , <b>2015</b> , 6, 8517	17.4	22
241	Single layer lead iodide: computational exploration of structural, electronic and optical properties, strain induced band modulation and the role of spin-orbital-coupling. <i>Nanoscale</i> , <b>2015</b> , 7, 15168-74	7.7	67
240	Evolution of Ni nanofilaments and electromagnetic coupling in the resistive switching of NiO. <i>Nanoscale</i> , <b>2015</b> , 7, 642-9	7.7	43
239	Tuning surface Dirac valleys by strain in topological crystalline insulators. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	10
238	Time-reversal symmetry protected chiral interface states between quantum spin and quantum anomalous Hall insulators. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	15
237	Emergence of a Chern-insulating state from a semi-Dirac dispersion. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	45
236	Converting normal insulators into topological insulators via tuning orbital levels. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	17
235	Tunable magnetic interaction in hydrogenated epitaxial graphene modulated by the SiC substrate. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	3
234	Band Engineering of Dirac Surface States in Topological-Insulator-Based van der Waals Heterostructures. <i>Physical Review Letters</i> , <b>2015</b> , 115, 136801	7.4	27
233	Effects of ferroelectric polarization on surface phase diagram: Evolutionary algorithm study of the BaTiO <sub>3</sub> (001) surface. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	12
232	Effects of strain and oxygen vacancies on the ferroelectric and antiferrodistortive distortions in PbTiO <sub>3</sub> /SrTiO <sub>3</sub> superlattice. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	33
231	Theory of the Dirac half metal and quantum anomalous Hall effect in Mn-intercalated epitaxial graphene. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	41
230	Predicted energetics and properties of rare-earth ferrites films grown on cubic (111)- and hexagonal (0001)-oriented substrates. <i>Journal of Physics Condensed Matter</i> , <b>2015</b> , 27, 485901	1.8	5
229	Quantum Unfolding: A program for unfolding electronic energy bands of materials. <i>Computer Physics Communications</i> , <b>2015</b> , 189, 213-219	4.2	13

228	Tailoring Native Defects and Zinc Impurities in Li <sub>4</sub> Ti <sub>5</sub> O <sub>12</sub> : Insights from First-Principles Study. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 5238-5245	3.8	19
227	Quantum thermal transport and spin thermoelectrics in low-dimensional nano systems: application of nonequilibrium Green's function method. <i>Wuli Xuebao/Acta Physica Sinica</i> , <b>2015</b> , 64, 186302	0.6	11
226	Thermal and thermoelectric properties of graphene. <i>Small</i> , <b>2014</b> , 10, 2182-99	11	183
225	Experimental observation of Dirac-like surface states and topological phase transition in Pb(1-x)Sn(x)Te(111) films. <i>Physical Review Letters</i> , <b>2014</b> , 112, 186801	7.4	91
224	Spin-filtered edge states with an electrically tunable gap in a two-dimensional topological crystalline insulator. <i>Nature Materials</i> , <b>2014</b> , 13, 178-83	27	230
223	Nontrivial Z <sub>2</sub> topology in bismuth-based III-V compounds. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	29
222	Weak topological insulators induced by the interlayer coupling: A first-principles study of stacked Bi <sub>2</sub> Te <sub>3</sub> . <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	43
221	Tunable anisotropic thermal conduction in graphene nanoribbons. <i>Applied Physics Letters</i> , <b>2014</b> , 104, 143108	3.4	13
220	High-rate, ultralong cycle-life lithium/sulfur batteries enabled by nitrogen-doped graphene. <i>Nano Letters</i> , <b>2014</b> , 14, 4821-7	11.5	615
219	First-principles study of 180° domain walls in BaTiO <sub>3</sub> : Mixed Bloch-Néel-Ising character. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	32
218	Giant room-temperature spin caloritronics in spin-semiconducting graphene nanoribbons. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	67
217	Functionalized germanene as a prototype of large-gap two-dimensional topological insulators. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	182
216	Anomalous properties of antiferroelectric PbZrO <sub>3</sub> under hydrostatic pressure. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	7
215	Microscopic origin of the p-type conductivity of the topological crystalline insulator SnTe and the effect of Pb alloying. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	70
214	Weak topological insulators in PbTe/SnTe superlattices. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	37
213	Manipulating topological phase transition by strain. <i>Acta Crystallographica Section C, Structural Chemistry</i> , <b>2014</b> , 70, 118-22	0.8	25
212	Chemical-potential-dependent gap opening at the Dirac surface states of Bi <sub>2</sub> Se <sub>3</sub> induced by aggregated substitutional Cr atoms. <i>Physical Review Letters</i> , <b>2014</b> , 112, 056801	7.4	84
211	Sulfur immobilization and lithium storage on defective graphene: A first-principles study. <i>Applied Physics Letters</i> , <b>2014</b> , 104, 043901	3.4	18

210	Publisher's Note: Chemical-Potential-Dependent Gap Opening at the Dirac Surface States of Bi <sub>2</sub> Se <sub>3</sub> Induced by Aggregated Substitutional Cr Atoms [Phys. Rev. Lett. 112, 056801 (2014)]. <i>Physical Review Letters</i> , <b>2014</b> , 112,	7.4	2
209	Anomalous properties of hexagonal rare-earth ferrites from first principles. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	40
208	Stable two-dimensional dumbbell stanene: A quantum spin Hall insulator. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	135
207	Topological crystalline insulator Pb <sub>x</sub> Sn <sub>1-x</sub> Te thin films on SrTiO <sub>3</sub> (001) with tunable Fermi levels. <i>APL Materials</i> , <b>2014</b> , 2, 056106	5.7	13
206	Thermal transport along Bi <sub>2</sub> Te <sub>3</sub> topological insulator nanowires. <i>Applied Physics Letters</i> , <b>2014</b> , 105, 023904	9.4	14
205	Realizing the quantum anomalous Hall effect in materials with in-plane magnetization. <i>National Science Review</i> , <b>2014</b> , 1, 33-33	10.8	
204	A general group theoretical method to unfold band structures and its application. <i>New Journal of Physics</i> , <b>2014</b> , 16, 033034	2.9	28
203	Structural stability and topological surface states of the SnTe (111) surface. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	27
202	Interfacial thermal conductance of partially unzipped carbon nanotubes: Linear scaling and exponential decay. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	26
201	Metallicity retained by covalent functionalization of graphene with phenyl groups. <i>Nanoscale</i> , <b>2013</b> , 5, 7537-43	7.7	7
200	Large-gap quantum spin Hall insulators in tin films. <i>Physical Review Letters</i> , <b>2013</b> , 111, 136804	7.4	952
199	Electronic structure of silicene on Ag(111): Strong hybridization effects. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	169
198	Topological insulators in transition-metal intercalated graphene: The role of d electrons in significantly increasing the spin-orbit gap. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	38
197	Field-effect birefringent spin lens in ultrathin film of magnetically doped topological insulators. <i>Physical Review Letters</i> , <b>2013</b> , 111, 116601	7.4	15
196	Comment on "Structural and electronic properties of T graphene: a two-dimensional carbon allotrope with tetrahedrings". <i>Physical Review Letters</i> , <b>2013</b> , 110, 029603	7.4	31
195	Improving the optical absorption of BiFeO <sub>3</sub> for photovoltaic applications via uniaxial compression or biaxial tension. <i>Applied Physics Letters</i> , <b>2013</b> , 102, 072905	3.4	44
194	Photon-assisted thermoelectric properties of noncollinear spin valves. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	34
193	Toward single-layer uniform hexagonal boron nitride-graphene patchworks with zigzag linking edges. <i>Nano Letters</i> , <b>2013</b> , 13, 3439-43	11.5	216

192	Elastic properties of tetragonal BiFeO <sub>3</sub> from first-principles calculations. <i>Applied Physics Letters</i> , <b>2013</b> , 102, 182905	3.4	36
191	The existence/absence of Dirac cones in graphynes. <i>New Journal of Physics</i> , <b>2013</b> , 15, 023004	2.9	87
190	Topology-driven magnetic quantum phase transition in topological insulators. <i>Science</i> , <b>2013</b> , 339, 1582-633	3.3	173
189	Tuning thermal conduction via extended defects in graphene. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	43
188	First-principles calculations on the effect of doping and biaxial tensile strain on electron-phonon coupling in graphene. <i>Physical Review Letters</i> , <b>2013</b> , 111, 196802	7.4	142
187	Interlayer interactions in graphites. <i>Scientific Reports</i> , <b>2013</b> , 3, 3046	4.9	138
186	Identifying Dirac cones in carbon allotropes with square symmetry. <i>Journal of Chemical Physics</i> , <b>2013</b> , 139, 184701	3.9	25
185	Two types of surface states in topological crystalline insulators. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	155
184	Edge stability of boron nitride nanoribbons and its application in designing hybrid BNC structures. <i>Nano Research</i> , <b>2012</b> , 5, 62-72	10	58
183	Electronic strengthening of graphene by charge doping. <i>Physical Review Letters</i> , <b>2012</b> , 109, 226802	7.4	91
182	Dirac fermions in strongly bound graphene systems. <i>Physical Review Letters</i> , <b>2012</b> , 109, 206802	7.4	44
181	High-resolution x-ray absorption studies of core excitons in hexagonal boron nitride. <i>Applied Physics Letters</i> , <b>2012</b> , 101, 191604	3.4	13
180	Role of Ga-doping in iron-gallium alloy clusters. <i>Chinese Physics B</i> , <b>2012</b> , 21, 027104	1.2	1
179	Electronic and magnetic properties of boron nitride nanoribbons with topological line defects. <i>RSC Advances</i> , <b>2012</b> , 2, 6192	3.7	14
178	Structural transition of large lead monoxide clusters. <i>Computational and Theoretical Chemistry</i> , <b>2012</b> , 983, 61-64	2	3
177	Enhancement of thermoelectric properties in graphene nanoribbons modulated with stub structures. <i>Applied Physics Letters</i> , <b>2012</b> , 100, 073105	3.4	67
176	Topological crystalline insulators in the SnTe material class. <i>Nature Communications</i> , <b>2012</b> , 3, 982	17.4	901
175	Topological and electronic transitions in a Sb(111) nanofilm: The interplay between quantum confinement and surface effect. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	146

174	Robust linear dependence of thermal conductance on radial strain in carbon nanotubes. <i>New Journal of Physics</i> , <b>2012</b> , 14, 013053	2.9	18
173	Manipulating stored images with phase imprinting at low light levels. <i>Optics Letters</i> , <b>2012</b> , 37, 2853-5	3	5
172	First-principles study of hydrogenated carbon nanotubes: A promising route for bilayer graphene nanoribbons. <i>Applied Physics Letters</i> , <b>2012</b> , 101, 033105	3.4	7
171	Interface engineering of epitaxial graphene on SiC(0001 $\bar{1}$ ) via fluorine intercalation: A first principles study. <i>Applied Physics Letters</i> , <b>2012</b> , 100, 103105	3.4	13
170	Design of strain-engineered quantum tunneling devices for topological surface states. <i>Applied Physics Letters</i> , <b>2012</b> , 100, 131602	3.4	23
169	Graphene oxide as a sulfur immobilizer in high performance lithium/sulfur cells. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 18522-5	16.4	1303
168	Ab initio Study of Half-Metallicity and Magnetism of Complex Organometallic Molecular Wires. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 7292-7297	3.8	15
167	All-optical Fresnel lens in coherent media: controlling image with image. <i>Optics Express</i> , <b>2011</b> , 19, 981-933	3.3	9
166	Slow-light-enhanced codirectional couplers with negative index materials. <i>Optics Express</i> , <b>2011</b> , 19, 10083-1013	3.3	1
165	Electronic and magnetic properties of early transition-metal substituted iron-cyclopentadienyl sandwich molecular wires: parity-dependent half-metallicity. <i>Journal of Chemical Physics</i> , <b>2011</b> , 135, 014702	3.0	3
164	Exciton in twisted single-walled carbon nanotube. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , <b>2011</b> , 8, 1190-1193		
163	Adsorption of DNA/RNA nucleobases on hexagonal boron nitride sheet: an ab initio study. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 12225-30	3.6	84
162	Formation, Morphology, and Effect of Complex Defects in Boron Nitride Nanotubes: An ab initio Calculation. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 12782-12788	3.8	7
161	Structural defects and electronic properties of the Cu-doped topological insulator Bi <sub>2</sub> Se <sub>3</sub> . <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	62
160	Lithium Intercalation Induced Decoupling of Epitaxial Graphene on SiC(0001): Electronic Property and Dynamic Process. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 23992-23997	3.8	27
159	Stable nontrivial Z <sub>2</sub> topology in ultrathin Bi (111) films: a first-principles study. <i>Physical Review Letters</i> , <b>2011</b> , 107, 136805	7.4	253
158	Generation of tunable-volume transmission-holographic gratings at low light levels. <i>Physical Review A</i> , <b>2011</b> , 84,	2.6	17
157	Trends in charge transfer and spin alignment of metallocene on graphene. <i>Physical Review B</i> , <b>2011</b> , 83,	3.3	14

156	Thermal transport by phonons in zigzag graphene nanoribbons with structural defects. <i>Journal of Physics Condensed Matter</i> , <b>2011</b> , 23, 315302	1.8	50
155	Beryllium-dihydrogen complexes on nanostructures. <i>Applied Physics Letters</i> , <b>2010</b> , 96, 143120	3.4	13
154	Optimizing photoelectrochemical properties of TiO <sub>2</sub> by chemical codoping. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	57
153	All-optical beam control with high speed using image-induced blazed gratings in coherent media. <i>Physical Review A</i> , <b>2010</b> , 82,	2.6	49
152	Releasing H <sub>2</sub> molecules with a partial pressure difference without the use of temperature. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	2
151	Quantized thermal conductance at low temperatures in quantum wire with catenoidal contacts. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	39
150	Electronic phase diagram of single-element silicon "strain" superlattices. <i>Physical Review Letters</i> , <b>2010</b> , 105, 016802	7.4	54
149	Orientation-dependent charge carrier confinement in a nanopatterned silicon film. <i>Applied Physics Letters</i> , <b>2010</b> , 97, 092116	3.4	
148	Multiple localized states and magnetic orderings in partially open zigzag carbon nanotube superlattices: an ab initio study. <i>Journal of Chemical Physics</i> , <b>2010</b> , 133, 084702	3.9	11
147	The half-metallicity of zigzag graphene nanoribbons with asymmetric edge terminations. <i>Journal of Nanoscience and Nanotechnology</i> , <b>2010</b> , 10, 5374-8	1.3	14
146	Thermal transport in graphene junctions and quantum dots. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	86
145	Intrinsic half-metallic BN nanotubes. <i>Applied Physics Letters</i> , <b>2010</b> , 97, 043115	3.4	52
144	Ab initio study of beryllium-decorated fullerenes for hydrogen storage. <i>Journal of Applied Physics</i> , <b>2010</b> , 107, 084304	2.5	20
143	A Chemical Modification Strategy for Hydrogen Storage in Covalent Organic Frameworks. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 13402-13407	3.8	32
142	Effects of hydrostatic pressure on Pb(Zr <sub>1-x</sub> Ti <sub>x</sub> )O <sub>3</sub> near the morphotropic phase boundary. <i>Journal of Applied Physics</i> , <b>2010</b> , 108, 124102	2.5	13
141	Spontaneous edge-defect formation and defect-induced conductance suppression in graphene nanoribbons. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	40
140	Hydrogen storage in Ca-decorated, B-substituted metal organic framework. <i>International Journal of Hydrogen Energy</i> , <b>2010</b> , 35, 198-203	6.7	34
139	Hydrogen-induced metallicity of SrTiO <sub>3</sub> (001) surfaces: A density functional theory study. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	40

- 138 Structural and electronic properties of Ge-Si, Sn-Si, and Pb-Si dimers on Si(001) from density-functional calculations. *Physical Review B*, **2009**, 79, 3-3 1
- 137 Intrinsic anisotropy of thermal conductance in graphene nanoribbons. *Applied Physics Letters*, **2009**, 95, 233116 3-4 158
- 136 Local vibrational excitation through extended electronic states at a germanium surface. *Physical Review Letters*, **2009**, 103, 266102 7-4 12
- 135 Preparing spin-polarized scanning tunneling microscope probes on capped carbon nanotubes by Fe doping: A first-principles study. *Applied Physics Letters*, **2009**, 94, 193106 3-4 4
- 134 Edge States of Zigzag Boron Nitride Nanoribbons. *Journal of the Physical Society of Japan*, **2009**, 78, 074713 26
- 133 Towards graphene nanoribbon-based electronics. *Frontiers of Physics in China*, **2009**, 4, 269-279 38
- 132 Flip motion of heterogeneous buckled dimers on Ge(001) by electron injection from STM tip. *Surface Science*, **2009**, 603, 781-787 1.8 2
- 131 Molecular and atomic adsorption of hydrogen on TiO<sub>2</sub> nanotubes: An ab initio study. *Chemical Physics Letters*, **2009**, 475, 82-85 2.5 55
- 130 Narrowed bandgaps and stronger excitonic effects from small boron nitride nanotubes. *Chemical Physics Letters*, **2009**, 476, 240-243 2.5 23
- 129 Activated dissociation of O<sub>2</sub> on Pb(111) surfaces by Pb adatoms. *Physical Review B*, **2009**, 80, 3-3 7
- 128 Quantum manifestations of graphene edge stress and edge instability: a first-principles study. *Physical Review Letters*, **2009**, 102, 166404 7-4 212
- 127 Ferromagnetism in pure wurtzite zinc oxide. *Journal of Applied Physics*, **2009**, 105, 07C508 2.5 84
- 126 Electronic and magnetic properties of partially open carbon nanotubes. *Journal of the American Chemical Society*, **2009**, 131, 17919-25 16.4 43
- 125 Magnetism of C adatoms on BN nanostructures: implications for functional nanodevices. *Journal of the American Chemical Society*, **2009**, 131, 1796-801 16.4 78
- 124 Half metallicity along the edge of zigzag boron nitride nanoribbons. *Physical Review B*, **2008**, 78, 3-3 211
- 123 Scattering potentials at Si-Ge and Sn-Ge impurity dimers on Ge(001) studied by scanning tunneling microscopy and ab initio calculations. *Physical Review B*, **2008**, 78, 3-3 2
- 122 Nonequilibrium Green's function method for phonon-phonon interactions and ballistic-diffusive thermal transport. *Physical Review B*, **2008**, 78, 3-3 79
- 121 Probing superexchange interaction in molecular magnets by spin-flip spectroscopy and microscopy. *Physical Review Letters*, **2008**, 101, 197208 7-4 210

120	Alkali-Metal-Doped B80 as High-Capacity Hydrogen Storage Media. <i>Journal of Physical Chemistry C</i> , <b>2008</b> , 112, 19268-19271	3.8	96
119	Hydrogen storage in alkali-metal-decorated organic molecules. <i>Applied Physics Letters</i> , <b>2008</b> , 93, 063107	3.4	26
118	Role of symmetry in the transport properties of graphene nanoribbons under bias. <i>Physical Review Letters</i> , <b>2008</b> , 100, 206802	7.4	387
117	Adsorption of Gas Molecules on Graphene Nanoribbons and Its Implication for Nanoscale Molecule Sensor. <i>Journal of Physical Chemistry C</i> , <b>2008</b> , 112, 13442-13446	3.8	430
116	Suppression of spin polarization in graphene nanoribbons by edge defects and impurities. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	169
115	Electron emission originated from free-electron-like states of alkali-doped boron-nitride nanotubes. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 17012-5	16.4	19
114	Scaling law of the giant Stark effect in boron nitride nanoribbons and nanotubes. <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	84
113	Theoretical investigation of the negative differential resistance in squashed C60 molecular device. <i>Applied Physics Letters</i> , <b>2008</b> , 92, 263304	3.4	94
112	Transverse pressure induced phase transitions in boron nitride nanotube bundles and the lightest boron nitride crystal. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 5257-61	16.4	31
111	Phase diagram of ferroelectric BaTiO <sub>3</sub> ultrathin films under open-circuit conditions. <i>Journal of Physics Condensed Matter</i> , <b>2008</b> , 20, 135203	1.8	10
110	The adsorption of O <sub>2</sub> on Pb films and the effect of quantum modulation: a first-principles prediction. <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 164705	3.9	19
109	Room-temperature dissociative hydrogen chemisorption on boron-doped fullerenes. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	18
108	Hydrogen-induced metallization of zinc oxide (211̄0) surface and nanowires: The effect of curvature. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	36
107	High-resolution scanning tunneling spectroscopy of magnetic impurity induced bound states in the superconducting gap of Pb thin films. <i>Physical Review Letters</i> , <b>2008</b> , 100, 226801	7.4	137
106	TUNABLE ELECTRIC CONDUCTIVITIES OF Au-DOPED BORON NITRIDE NANOTUBES. <i>Nano</i> , <b>2007</b> , 02, 367-372	1.1	3
105	Intrinsic current-voltage characteristics of graphene nanoribbon transistors and effect of edge doping. <i>Nano Letters</i> , <b>2007</b> , 7, 1469-73	11.5	512
104	CO methanation on Ni(1 1 1) and modified Ni <sub>3</sub> Al(1 1 1) surfaces: A first-principle study. <i>Surface Science</i> , <b>2007</b> , 601, 475-478	1.8	12
103	Spin-polarized electron current from carbon-doped open armchair boron nitride nanotubes: Implication for nano-spintronic devices. <i>Chemical Physics Letters</i> , <b>2007</b> , 437, 83-86	2.5	22

102	Study of dissociation barriers of on and. <i>Physica B: Condensed Matter</i> , <b>2007</b> , 393, 223-227	2.8	8
101	Experimental observation of quantum oscillation of surface chemical reactivities. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2007</b> , 104, 9204-8	11.5	113
100	Unusual vortex structure in ultrathin Pb(Zr <sub>0.5</sub> Ti <sub>0.5</sub> )O <sub>3</sub> films. <i>Journal of Applied Physics</i> , <b>2007</b> , 101, 014112	5	14
99	Structures and stabilities of small lead oxide clusters Pb <sub>m</sub> O <sub>n</sub> (m=1-4,n=1-2m). <i>Journal of Chemical Physics</i> , <b>2007</b> , 126, 134705	3.9	16
98	Self-organization nanodomain structure in ferroelectric ultrathin films. <i>Nanotechnology</i> , <b>2007</b> , 18, 325703	3.4	7
97	Quantum confinement of crystalline silicon nanotubes with nonuniform wall thickness: Implication to modulation doping. <i>Applied Physics Letters</i> , <b>2007</b> , 91, 103107	3.4	10
96	Structural and electronic properties of fluorinated double-walled boron nitride nanotubes: Effect of interwall interaction. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	20
95	Manipulating the Kondo resonance through quantum size effects. <i>Physical Review Letters</i> , <b>2007</b> , 99, 256601	3.4	187
94	Making a field effect transistor on a single graphene nanoribbon by selective doping. <i>Applied Physics Letters</i> , <b>2007</b> , 91, 253122	3.4	146
93	Physical mechanism of transport blocking in metallic zigzag carbon nanotubes. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	17
92	Oxidation of carbon monoxide on Rh(111): a density functional theory study. <i>Journal of Chemical Physics</i> , <b>2006</b> , 124, 234703	3.9	18
91	Effects of vacancy-carboxyl pair functionalization on electronic properties of carbon nanotubes. <i>Applied Physics Letters</i> , <b>2006</b> , 89, 173130	3.4	41
90	Coadsorption of potassium and carbon monoxide on Ni(111): A density functional theory study. <i>Physical Review B</i> , <b>2006</b> , 74,	3.3	10
89	Modulating transmission properties of nanoscale transistors by dipoles near contacts. <i>Applied Physics Letters</i> , <b>2006</b> , 89, 243106	3.4	
88	Mechanism of nanoelectronic switch based on telescoping carbon nanotubes. <i>Applied Physics Letters</i> , <b>2006</b> , 88, 173107	3.4	41
87	Bonding modes and electronic properties of single-crystalline silicon nanotubes. <i>Physical Review B</i> , <b>2006</b> , 73,	3.3	17
86	Chemical functionalization of carbon nanotubes by carboxyl groups on stone-wales defects: a density functional theory study. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 10266-71	3.4	115
85	Uniaxial-stress effects on electronic properties of silicon carbide nanowires. <i>Applied Physics Letters</i> , <b>2006</b> , 89, 023104	3.4	37

84	Structural, electronic, and magnetic properties of manganese-doped Zn <sub>12</sub> O <sub>12</sub> clusters: a first-principles study. <i>Journal of Chemical Physics</i> , <b>2006</b> , 124, 174705	3.9	40
83	Hydrostatic-pressure-induced porous gallium nitride from nanotube bundles: an ab initio study. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 174711	3.9	2
82	Tremendous spin-splitting effects in open boron nitride nanotubes: application to nanoscale spintronic devices. <i>Journal of the American Chemical Society</i> , <b>2006</b> , 128, 8453-8	16.4	82
81	Theoretical modeling and simulations of perovskite ferroelectrics: From phenomenological approaches to ab initio. <i>Current Opinion in Solid State and Materials Science</i> , <b>2006</b> , 10, 40-51	12	16
80	Atomic-vacancy effects on field electron emission of carbon nanotubes: A first-principles study. <i>Chemical Physics Letters</i> , <b>2006</b> , 423, 229-233	2.5	5
79	Selective adsorption of first-row atoms on BN nanotubes. <i>Chemical Physics Letters</i> , <b>2006</b> , 426, 148-154	2.5	27
78	Localized mixed acoustic modes in non-cubic-axial superlattice with a cap layer. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2006</b> , 31, 57-61	3	2
77	Study of structure characteristics of the Ga <sub>8</sub> As <sub>8</sub> cluster. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2006</b> , 349, 224-229	2.3	12
76	Effect of defects on the thermal conductivity in a nanowire. <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	93
75	Long-range interaction between Stone-Wales defects in zigzag single-walled carbon nanotubes. <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	9
74	Structural characterizations and electronic properties of boron nitride nanotube crystalline bundles. <i>Journal of Chemical Physics</i> , <b>2005</b> , 123, 124716	3.9	18
73	Spin-polarized electron current from Mn-doped closed zigzag GaN nanotubes. <i>Chemical Physics Letters</i> , <b>2005</b> , 401, 47-51	2.5	6
72	Structural trends interpretation of the metal-to-semiconductor transition in deformed carbon nanotubes. <i>Journal of Applied Physics</i> , <b>2005</b> , 97, 114314	2.5	10
71	Field emission in doped nanotubes. <i>Journal of Nanoscience and Nanotechnology</i> , <b>2005</b> , 5, 1421-34	1.3	31
70	Long periodic oscillation of electronic properties in capped finite-length armchair carbon nanotubes. <i>Physical Review B</i> , <b>2005</b> , 71,	3.3	6
69	Generation of narrow-band terahertz radiation with preset frequency components in poled ferroelectric materials. <i>Journal of Applied Physics</i> , <b>2005</b> , 97, 114108	2.5	4
68	Phase diagram of ultrathin Pb(Zr <sub>0.5</sub> Ti <sub>0.5</sub> )O <sub>3</sub> films under strain. <i>Applied Physics Letters</i> , <b>2005</b> , 86, 202903	3.4	13
67	Ab initio study of transport properties of multiwalled carbon nanotubes. <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	46

66	Dielectric properties of relaxor ferroelectric films. <i>Journal of Applied Physics</i> , <b>2005</b> , 98, 094105	2.5	6
65	Spontaneous polarizations of ultrashort-period epitaxial KNbO <sub>3</sub> (KTaO <sub>3</sub> ) <sub>m</sub> superlattices: An ab initio investigation. <i>Applied Physics Letters</i> , <b>2005</b> , 86, 232903	3.4	18
64	Physical origin of hydrogen-adsorption-induced metallization of the SiC surface: n-type doping via formation of hydrogen bridge bond. <i>Physical Review Letters</i> , <b>2005</b> , 95, 196803	7.4	28
63	Effects of finite deformed length in carbon nanotubes. <i>Applied Physics Letters</i> , <b>2004</b> , 84, 4203-4205	3.4	21
62	Electronic-structure theory of crystalline insulators under a homogeneous electric field. <i>Physical Review B</i> , <b>2004</b> , 69,	3.3	6
61	Theoretical studies on the electronic structure of Ti <sub>8</sub> C <sub>12</sub> isomers. <i>Journal of Chemical Physics</i> , <b>2004</b> , 121, 4123-6	3.9	5
60	Electronic states and doping effect of carbon in the edge-dislocation core of bcc iron. <i>Physical Review B</i> , <b>2004</b> , 69,	3.3	23
59	Spin-polarized electron emitter: Mn-doped GaN nanotubes and their arrays. <i>Physical Review B</i> , <b>2004</b> , 69,	3.3	31
58	Ferroelectricity in Pb(Zr <sub>0.5</sub> Ti <sub>0.5</sub> )O <sub>3</sub> thin films: Critical thickness and 180° stripe domains. <i>Physical Review B</i> , <b>2004</b> , 70,	3.3	39
57	Tunneling energy barriers of emitted electrons in single-walled carbon nanotubes. <i>Physical Review B</i> , <b>2004</b> , 70,	3.3	4
56	Electronic transport mechanism of a molecular electronic device: structural effects and terminal atoms. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2004</b> , 323, 154-158	2.3	35
55	Acoustic phonon mode splitting behavior of an asymmetric y-branch three terminal junction. <i>Applied Physics Letters</i> , <b>2004</b> , 85, 822-824	3.4	52
54	Single electron emission from the closed-tips of single-walled carbon nanotubes. <i>Journal of Chemical Physics</i> , <b>2004</b> , 121, 12600-5	3.9	6
53	Structural and electronic properties of n-doped and p-doped SrTiO <sub>3</sub> . <i>Physical Review B</i> , <b>2004</b> , 70,	3.3	118
52	Acoustic phonon transport through a T-shaped quantum waveguide. <i>Journal of Physics Condensed Matter</i> , <b>2004</b> , 16, 5049-5059	1.8	42
51	A comprehensive study of Heisenberg-like systems with internal spin fluctuation. <i>Journal of Physics Condensed Matter</i> , <b>2003</b> , 15, 2783-2796	1.8	9
50	Effect of tunneling frequency on relaxor behavior. <i>Microelectronic Engineering</i> , <b>2003</b> , 66, 676-682	2.5	3
49	Influence of the structural defects on localized interface optical-phonon modes in periodically layered heterostructures. <i>Microelectronic Engineering</i> , <b>2003</b> , 66, 26-32	2.5	

48	Impact of structural defects on the localized acoustic wave in superlattices. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2003</b> , 308, 285-293	2.3	7
47	Phonon transport and thermal conductivity in dielectric quantum wire. <i>Journal Physics D: Applied Physics</i> , <b>2003</b> , 36, 3027-3033	3	50
46	Huge enhancement of electromechanical responses in compositionally modulated Pb(Zr(1-x)Ti <sub>x</sub> )O <sub>3</sub> . <i>Physical Review Letters</i> , <b>2003</b> , 91, 067602	7.4	27
45	Metal-to-semiconductor transition in squashed armchair carbon nanotubes. <i>Physical Review Letters</i> , <b>2003</b> , 90, 156601	7.4	124
44	Effect of defect-induced internal field on the aging of relaxors. <i>Physical Review B</i> , <b>2003</b> , 67,	3.3	20
43	Localized interface optical-phonon modes in two coupled semi-infinite superlattices. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2002</b> , 299, 634-643	2.3	30
42	The effects of oxygen substitution on electronic structure of single-walled carbon nanotubes. <i>Solid State Communications</i> , <b>2002</b> , 122, 121-124	1.6	8
41	Emission probabilities of electrons in carbon nanotubes. <i>Applied Physics Letters</i> , <b>2002</b> , 80, 1999-2001	3.4	12
40	First-principles study of the stability of the icosahedral Ti <sub>13</sub> , Ti <sub>13</sub> <sup>+</sup> , and Ti <sub>13</sub> +1 clusters. <i>Physical Review B</i> , <b>2002</b> , 65,	3.3	39
39	Effect of substitutional atoms in the tip on field-emission properties of capped carbon nanotubes. <i>Applied Physics Letters</i> , <b>2002</b> , 80, 2589-2591	3.4	69
38	Qualitative and quantitative descriptions on the localized electronic structure in single-walled carbon nanotubes. <i>Journal of Chemical Physics</i> , <b>2002</b> , 116, 2284-2288	3.9	5
37	Multiple tunneling channels order-disorder ferroelectric model and field-induced phase transition in relaxors. <i>Physical Review B</i> , <b>2002</b> , 65,	3.3	7
36	First-principles investigation into the structural stability of icosahedral Ti <sub>12</sub> X clusters (X = B, C, N, Al, Si, P, V, Cr, Mn, Fe, Co and Ni). <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , <b>2002</b> , 35, 4015-4019	1.3	6
35	Localized interface optical phonon modes in a semi-infinite superlattice with a cap layer. <i>Journal of Physics Condensed Matter</i> , <b>2002</b> , 14, 13761-13775	1.8	14
34	Ab initio study of MgSiO <sub>3</sub> low-clinoenstatite at high pressure. <i>American Mineralogist</i> , <b>2001</b> , 86, 762-766	2.9	5
33	Stochastic resonance induced by random fields in ferroelectrics. <i>Europhysics Letters</i> , <b>2001</b> , 55, 1-5	1.6	9
32	First-principles study on morphology and mechanical properties of single-walled carbon nanotube. <i>Chemical Physics Letters</i> , <b>2001</b> , 333, 344-349	2.5	149
31	Electronic structure and field-emission characteristics of open-ended single-walled carbon nanotubes. <i>Physical Review Letters</i> , <b>2001</b> , 87, 095504	7.4	114

- 30 Dimensional effects on field emission properties of the body for single-walled carbon nanotube. *Applied Physics Letters*, **2001**, 79, 836-838 3-4 41
- 29 Proposed measurement of coherence and phase sensitivity in a mesoscopic system. *Physical Review B*, **2001**, 63, 3-3 1
- 28 Soft modes in order-disorder ferroelectrics. *Applied Physics Letters*, **2001**, 79, 1333-1335 3-4 2
- 27 Energetics and electronic structure of Re and Ta in the  $\gamma$  phase of Ni-based superalloys. *Physical Review B*, **2001**, 65, 3-3 42
- 26 Ab initio structure of MgSiO<sub>3</sub> ilmenite at high pressure. *American Mineralogist*, **2000**, 85, 317-320 2.9 12
- 25 Electron-optical-phonon scattering in non-square quantum-well structures. *Solid State Communications*, **2000**, 114, 101-106 1.6 5
- 24 Finite size effects in carbon nanotubes. *Applied Physics Letters*, **2000**, 77, 2554-2556 3-4 25
- 23 Magnetostructural effects and phase transition in Cr<sub>2</sub>O<sub>3</sub> under pressure. *Physical Review B*, **2000**, 62, 11997-12000 3-3 22
- 22 First-principles search for high-pressure phases of GaAsO<sub>4</sub>. *Physical Review B*, **1999**, 60, 3751-3756 3-3 5
- 21 High-pressure elasticity of alumina studied by first principles. *American Mineralogist*, **1999**, 84, 1961-1966 2.9 26
- 20 First-principles study of high-pressure alumina polymorphs. *Physical Review B*, **1998**, 57, 10363-10369 3-3 44
- 19 Optical Transitions in Ruby across the Corundum to Rh<sub>2</sub>O<sub>3</sub> (II) Phase Transformation. *Physical Review Letters*, **1998**, 81, 3267-3270 7-4 35
- 18 Resonant Tunneling in an Aharonov-Bohm Ring with a Quantum Dot. *Physical Review Letters*, **1998**, 80, 1952-1955 7-4 59
- 17 The Study on the Filling of Atoms in a Carbon Nanotube. *International Journal of Modern Physics B*, **1998**, 12, 1601-1606 1.1 7
- 16 Ruby's Optical Transitions: Effects of Pressure-Induced Phase Transformation. *Materials Research Society Symposia Proceedings*, **1997**, 499, 275 1
- 15 Transport in asymmetric multiple-barrier magnetic nanostructures. *Physical Review B*, **1997**, 55, 9314-9317 3-3 37
- 14 Level width of a quasibound state in a double-barrier parabolic-well resonant tunneling structure. *Zeitschrift für Physik B-Condensed Matter*, **1997**, 102, 217-221 5
- 13 Intrasubband electron-phonon scattering in doped thin-layer inserted quantum well. *Solid State Communications*, **1997**, 104, 689-694 1.6

12	Effect of an electric field on electron-interface-phonon scattering in a graded quantum well. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>1996</b> , 215, 309-316	2.3	1
11	Electric-field-dependent intersubband transition via optical phonons in a doped-thin-layer inserted quantum-well structure. <i>Physical Review B</i> , <b>1996</b> , 54, 16983-16988	3.3	10
10	A first principles interatomic potential and application to the grain boundary in Ni. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>1995</b> , 197, 449-457	2.3	4
9	Chemical composition fluctuations at interfaces in quantum well structures: effect on interface phonon modes. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>1995</b> , 200, 329-334	2.3	1
8	Optical Interface Phonon in Graded Quantum Well Structures. <i>Chinese Physics Letters</i> , <b>1994</b> , 11, 349-352	1.8	1
7	Electron-interface-phonon scattering in graded quantum wells of Ga <sub>1-x</sub> Al <sub>x</sub> As. <i>Physical Review B</i> , <b>1994</b> , 49, 14403-14408	3.3	19
6	Electron-phonon scattering in Ga <sub>1-x</sub> Al <sub>x</sub> As quantum-well structures in an electric field. <i>Physical Review B</i> , <b>1994</b> , 50, 5473-5479	3.3	10
5	Electron-interface phonon scattering in GaAs/Ga <sub>1-x</sub> Al <sub>x</sub> As quantum-well structures with interface roughness. <i>Journal of Physics Condensed Matter</i> , <b>1993</b> , 5, 2859-2868	1.8	16
4	D- centers in spherical quantum dots. <i>Physical Review B</i> , <b>1992</b> , 46, 7546-7550	3.3	51
3	A mechanism of structural transition in YBa <sub>2</sub> Cu <sub>3</sub> O <sub>7-<math>\delta</math></sub> . <i>Physica C: Superconductivity and Its Applications</i> , <b>1989</b> , 162-164, 1515-1516	1.3	
2	Realization of Coexisting Charge Density Wave and Quantum Spin/Anomalous Hall State in Monolayer NbTe <sub>2</sub> . <i>Advanced Functional Materials</i> , 2111675	15.6	3
1	Deep-learning density functional theory Hamiltonian for efficient ab initio electronic-structure calculation. <i>Nature Computational Science</i> ,		1