Wenhui Duan

List of Publications by Citations

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	Graphene oxide as a sulfur immobilizer in high performance lithium/sulfur cells. *Journal of the American Chemical Society*, **2011**, 133, 18522-5	16.4	1303
388	Large-gap quantum spin Hall insulators in tin films. *Physical Review Letters*, **2013**, 111, 136804	7.4	952
387	Topological crystalline insulators in the SnTe material class. *Nature Communications*, **2012**, 3, 982	17.4	901
386	High-rate, ultralong cycle-life lithium/sulfur batteries enabled by nitrogen-doped graphene. *Nano Letters*, **2014**, 14, 4821-7	11.5	615
385	Intrinsic current-voltage characteristics of graphene nanoribbon transistors and effect of edge doping. *Nano Letters*, **2007**, 7, 1469-73	11.5	512
384	Experimental observation of topological Fermi arcs in type-II Weyl semimetal MoTe2. *Nature Physics*, **2016**, 12, 1105-1110	16.2	506
383	Discovery of robust in-plane ferroelectricity in atomic-thick SnTe. *Science*, **2016**, 353, 274-8	33.3	470
382	Adsorption of Gas Molecules on Graphene Nanoribbons and Its Implication for Nanoscale Molecule Sensor. *Journal of Physical Chemistry C*, **2008**, 112, 13442-13446	3.8	430
381	Role of symmetry in the transport properties of graphene nanoribbons under bias. *Physical Review Letters*, **2008**, 100, 206802	7.4	387
380	Intrinsic magnetic topological insulators in van der Waals layered MnBiTe-family materials. *Science Advances*, **2019**, 5, eaaw5685	14.3	330
379	Experimental Realization of an Intrinsic Magnetic Topological Insulator*. *Chinese Physics Letters*, **2019**, 36, 076801	1.8	260
378	Stable nontrivial Z2 topology in ultrathin Bi (111) films: a first-principles study. *Physical Review Letters*, **2011**, 107, 136805	7.4	253
377	Lorentz-violating type-II Dirac fermions in transition metal dichalcogenide PtTe. *Nature Communications*, **2017**, 8, 257	17.4	239
376	Spin-filtered edge states with an electrically tunable gap in a two-dimensional topological crystalline insulator. *Nature Materials*, **2014**, 13, 178-83	27	230
375	Toward single-layer uniform hexagonal boron nitride-graphene patchworks with zigzag linking edges. *Nano Letters*, **2013**, 13, 3439-43	11.5	216
374	Quantum manifestations of graphene edge stress and edge instability: a first-principles study. *Physical Review Letters*, **2009**, 102, 166404	7.4	212
373	Half metallicity along the edge of zigzag boron nitride nanoribbons. *Physical Review B*, **2008**, 78,	3.3	211

372	Probing superexchange interaction in molecular magnets by spin-flip spectroscopy and microscopy. *Physical Review Letters*, **2008**, 101, 197208	7.4	210
371	Manipulating the Kondo resonance through quantum size effects. *Physical Review Letters*, **2007**, 99, 256601	7.4	187
370	Type-II Dirac fermions in the PtSe2 class of transition metal dichalcogenides. *Physical Review B*, **2016**, 94,	3.3	187
369	Thermal and thermoelectric properties of graphene. *Small*, **2014**, 10, 2182-99	11	183
368	Functionalized germanene as a prototype of large-gap two-dimensional topological insulators. *Physical Review B*, **2014**, 89,	3.3	182
367	Epitaxial growth of ultraflat stanene with topological band inversion. *Nature Materials*, **2018**, 17, 1081-1086	27	175
366	Topology-driven magnetic quantum phase transition in topological insulators. *Science*, **2013**, 339, 1582-6	33.3	173
365	Electronic structure of silicene on Ag(111): Strong hybridization effects. *Physical Review B*, **2013**, 88,	3.3	169
364	Suppression of spin polarization in graphene nanoribbons by edge defects and impurities. *Physical Review B*, **2008**, 77,	3.3	169
363	Tunable Structural, Electronic, and Optical Properties of Layered Two-Dimensional C2N and MoS2 van der Waals Heterostructure as Photovoltaic Material. *Journal of Physical Chemistry C*, **2017**, 121, 3654-3660	3.8	166
362	Topological nodal-line semimetals in alkaline-earth stannides, germanides, and silicides. *Physical Review B*, **2016**, 93,	3.3	160
361	Intrinsic anisotropy of thermal conductance in graphene nanoribbons. *Applied Physics Letters*, **2009**, 95, 233116	3.4	158
360	Two types of surface states in topological crystalline insulators. *Physical Review B*, **2013**, 88,	3.3	155
359	First-principles study on morphology and mechanical properties of single-walled carbon nanotube. *Chemical Physics Letters*, **2001**, 333, 344-349	2.5	149
358	Topological and electronic transitions in a Sb(111) nanofilm: The interplay between quantum confinement and surface effect. *Physical Review B*, **2012**, 85,	3.3	146
357	Making a field effect transistor on a single graphene nanoribbon by selective doping. *Applied Physics Letters*, **2007**, 91, 253122	3.4	146
356	Experimental evidence for type-II Dirac semimetal in PtSe2. *Physical Review B*, **2017**, 96,	3.3	142
355	First-principles calculations on the effect of doping and biaxial tensile strain on electron-phonon coupling in graphene. *Physical Review Letters*, **2013**, 111, 196802	7.4	142

354	Interlayer interactions in graphites. *Scientific Reports*, **2013**, 3, 3046	4.9	138
353	High-resolution scanning tunneling spectroscopy of magnetic impurity induced bound states in the superconducting gap of Pb thin films. *Physical Review Letters*, **2008**, 100, 226801	7.4	137
352	Stable two-dimensional dumbbell stanene: A quantum spin Hall insulator. *Physical Review B*, **2014**, 90,	3.3	135
351	Metal-to-semiconductor transition in squashed armchair carbon nanotubes. *Physical Review Letters*, **2003**, 90, 156601	7.4	124
350	Single-atom catalyst boosts electrochemical conversion reactions in batteries. *Energy Storage Materials*, **2019**, 18, 246-252	19.4	121
349	Structural and electronic properties of n-doped and p-doped SrTiO3. *Physical Review B*, **2004**, 70,	3.3	118
348	Chemical functionalization of carbon nanotubes by carboxyl groups on stone-wales defects: a density functional theory study. *Journal of Physical Chemistry B*, **2006**, 110, 10266-71	3.4	115
347	Electronic structure and field-emission characteristics of open-ended single-walled carbon nanotubes. *Physical Review Letters*, **2001**, 87, 095504	7.4	114
346	High quality atomically thin PtSe 2 films grown by molecular beam epitaxy. *2D Materials*, **2017**, 4, 045015	5.9	113
345	Experimental observation of quantum oscillation of surface chemical reactivities. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 9204-8	11.5	113
344	A few-layered Ti3C2 nanosheet/glass fiber composite separator as a lithium polysulphide reservoir for high-performance lithium–sulfur batteries. *Journal of Materials Chemistry A*, **2016**, 4, 5993-5998	13	112
343	Direct observation of spin-layer locking by local Rashba effect in monolayer semiconducting PtSe film. *Nature Communications*, **2017**, 8, 14216	17.4	110
342	Multifunctional Interlayer Based on Molybdenum Diphosphide Catalyst and Carbon Nanotube Film for Lithium-Sulfur Batteries. *Small*, **2018**, 14, 1702853	11	108
341	Scaling Universality between Band Gap and Exciton Binding Energy of Two-Dimensional Semiconductors. *Physical Review Letters*, **2017**, 118, 266401	7.4	107
340	Tunable Magnetism in Transition-Metal-Decorated Phosphorene. *Journal of Physical Chemistry C*, **2015**, 119, 10059-10063	3.8	96
339	Alkali-Metal-Doped B80 as High-Capacity Hydrogen Storage Media. *Journal of Physical Chemistry C*, **2008**, 112, 19268-19271	3.8	96
338	Theoretical investigation of the negative differential resistance in squashed C60 molecular device. *Applied Physics Letters*, **2008**, 92, 263304	3.4	94
337	Effect of defects on the thermal conductivity in a nanowire. *Physical Review B*, **2005**, 72,	3.3	93

336	Liquid-Phase Electrochemical Scanning Electron Microscopy for In Situ Investigation of Lithium Dendrite Growth and Dissolution. *Advanced Materials*, **2017**, 29, 1606187	24	91
335	Experimental observation of Dirac-like surface states and topological phase transition in Pb(1-x)Sn(x)Te(111) films. *Physical Review Letters*, **2014**, 112, 186801	7.4	91
334	Electronic strengthening of graphene by charge doping. *Physical Review Letters*, **2012**, 109, 226802	7.4	91
333	The existence/absence of Dirac cones in graphynes. *New Journal of Physics*, **2013**, 15, 023004	2.9	87
332	Scanning Tunneling Microscopy of the Magnetism of a Single Carbon Vacancy in Graphene. *Physical Review Letters*, **2016**, 117, 166801	7.4	87
331	Thermal transport in graphene junctions and quantum dots. *Physical Review B*, **2010**, 81,	3.3	86
330	Enhanced performance of lithium-sulfur batteries with an ultrathin and lightweight MoS2/carbon nanotube interlayer. *Journal of Power Sources*, **2018**, 389, 169-177	8.9	85
329	Chemical-potential-dependent gap opening at the Dirac surface states of Bi2Se3 induced by aggregated substitutional Cr atoms. *Physical Review Letters*, **2014**, 112, 056801	7.4	84
328	Adsorption of DNA/RNA nucleobases on hexagonal boron nitride sheet: an ab initio study. *Physical Chemistry Chemical Physics*, **2011**, 13, 12225-30	3.6	84
327	Ferromagnetism in pure wurtzite zinc oxide. *Journal of Applied Physics*, **2009**, 105, 07C508	2.5	84
326	Scaling law of the giant Stark effect in boron nitride nanoribbons and nanotubes. *Physical Review B*, **2008**, 78,	3.3	84
325	Tremendous spin-splitting effects in open boron nitride nanotubes: application to nanoscale spintronic devices. *Journal of the American Chemical Society*, **2006**, 128, 8453-8	16.4	82
324	Nonequilibrium Green function method for phonon-phonon interactions and ballistic-diffusive thermal transport. *Physical Review B*, **2008**, 78,	3.3	79
323	Magnetism of C adatoms on BN nanostructures: implications for functional nanodevices. *Journal of the American Chemical Society*, **2009**, 131, 1796-801	16.4	78
322	Microscopic origin of the p-type conductivity of the topological crystalline insulator SnTe and the effect of Pb alloying. *Physical Review B*, **2014**, 89,	3.3	70
321	Effect of substitutional atoms in the tip on field-emission properties of capped carbon nanotubes. *Applied Physics Letters*, **2002**, 80, 2589-2591	3.4	69
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319	Giant room-temperature spin caloritronics in spin-semiconducting graphene nanoribbons. *Physical Review B*, **2014**, 90,	3.3	67

318	Enhancement of thermoelectric properties in graphene nanoribbons modulated with stub structures. *Applied Physics Letters*, **2012**, 100, 073105	3.4	67
317	Molecular Beam Epitaxy-Grown SnSe in the Rock-Salt Structure: An Artificial Topological Crystalline Insulator Material. *Advanced Materials*, **2015**, 27, 4150-4	24	64
316	Model for topological phononics and phonon diode. *Physical Review B*, **2017**, 96,	3.3	63
315	Structural defects and electronic properties of the Cu-doped topological insulator Bi2Se3. *Physical Review B*, **2011**, 84,	3.3	62
314	Resonant Tunneling in an Aharonov-Bohm Ring with a Quantum Dot. *Physical Review Letters*, **1998**, 80, 1952-1955	7.4	59
313	Edge stability of boron nitride nanoribbons and its application in designing hybrid BNC structures. *Nano Research*, **2012**, 5, 62-72	10	58
312	Optimizing photoelectrochemical properties of TiO2 by chemical codoping. *Physical Review B*, **2010** , 82,	3.3	57
311	Unveiling Charge-Density Wave, Superconductivity, and Their Competitive Nature in Two-Dimensional NbSe. *Nano Letters*, **2018**, 18, 2924-2929	11.5	56
310	Molecular and atomic adsorption of hydrogen on TiO2 nanotubes: An ab initio study. *Chemical Physics Letters*, **2009**, 475, 82-85	2.5	55
309	Electronic phase diagram of single-element silicon "strain" superlattices. *Physical Review Letters*, **2010**, 105, 016802	7.4	54
308	Pseudospins and Topological Effects of Phonons in a Kekul□Lattice. *Physical Review Letters*, **2017**, 119, 255901	7.4	53
307	Intrinsic half-metallic BN□ nanotubes. *Applied Physics Letters*, **2010**, 97, 043115	3.4	52
306	Acoustic phonon mode splitting behavior of an asymmetric y-branch three terminal junction. *Applied Physics Letters*, **2004**, 85, 822-824	3.4	52
305	D- centers in spherical quantum dots. *Physical Review B*, **1992**, 46, 7546-7550	3.3	51
304	Thermal transport by phonons in zigzag graphene nanoribbons with structural defects. *Journal of Physics Condensed Matter*, **2011**, 23, 315302	1.8	50
303	Phonon transport and thermal conductivity in dielectric quantum wire. *Journal Physics D: Applied Physics*, **2003**, 36, 3027-3033	3	50
302	All-optical beam control with high speed using image-induced blazed gratings in coherent media. *Physical Review A*, **2010**, 82,	2.6	49
301	Universal Descriptor for Large-Scale Screening of High-Performance MXene-Based Materials for Energy Storage and Conversion. *Chemistry of Materials*, **2018**, 30, 2687-2693	9.6	47

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299	Magnetically controllable topological quantum phase transitions in the antiferromagnetic topological insulator MnBi2Te4. *Physical Review B*, **2019**, 100,	3.3	45
298	Emergence of a Chern-insulating state from a semi-Dirac dispersion. *Physical Review B*, **2015**, 92,	3.3	45
297	Improving the optical absorption of BiFeO3 for photovoltaic applications via uniaxial compression or biaxial tension. *Applied Physics Letters*, **2013**, 102, 072905	3.4	44
296	Dirac fermions in strongly bound graphene systems. *Physical Review Letters*, **2012**, 109, 206802	7.4	44
295	First-principles study of high-pressure alumina polymorphs. *Physical Review B*, **1998**, 57, 10363-10369	3.3	44
294	Evolution of Ni nanofilaments and electromagnetic coupling in the resistive switching of NiO. *Nanoscale*, **2015**, 7, 642-9	7.7	43
293	Weak topological insulators induced by the interlayer coupling: A first-principles study of stacked Bi2TeI. *Physical Review B*, **2014**, 89,	3.3	43
292	Tuning thermal conduction via extended defects in graphene. *Physical Review B*, **2013**, 87,	3.3	43
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289	Single atomic cobalt catalyst significantly accelerates lithium ion diffusion in high mass loading Li2S cathode. *Energy Storage Materials*, **2020**, 28, 375-382	19.4	42
288	Acoustic phonon transport through a T-shaped quantum waveguide. *Journal of Physics Condensed Matter*, **2004**, 16, 5049-5059	1.8	42
287	Energetics and electronic structure of Re and Ta in the □ phase of Ni-based superalloys. *Physical Review B*, **2001**, 65,	3.3	42
286	Theory of the Dirac half metal and quantum anomalous Hall effect in Mn-intercalated epitaxial graphene. *Physical Review B*, **2015**, 92,	3.3	41
285	Effects of vacancy-carboxyl pair functionalization on electronic properties of carbon nanotubes. *Applied Physics Letters*, **2006**, 89, 173130	3.4	41
284	Mechanism of nanoelectronic switch based on telescoping carbon nanotubes. *Applied Physics Letters*, **2006**, 88, 173107	3.4	41
283	Dimensional effects on field emission properties of the body for single-walled carbon nanotube. *Applied Physics Letters*, **2001**, 79, 836-838	3.4	41

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281	Anomalous properties of hexagonal rare-earth ferrites from first principles. *Physical Review B*, **2014**, 89,	3.3	40
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270	Towards graphene nanoribbon-based electronics. *Frontiers of Physics in China*, **2009**, 4, 269-279		38
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268	Weak topological insulators in PbTe/SnTe superlattices. *Physical Review B*, **2014**, 89,	3.3	37
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259	Two-dimensional ferromagnetic-ferroelectric multiferroics in violation of the d0 rule. *Physical Review B*, **2019**, 99,	3.3	34
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257	Hydrogen storage in Ca-decorated, B-substituted metal organic framework. *International Journal of Hydrogen Energy*, **2010**, 35, 198-203	6.7	34
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255	Electronic States and Magnetic Response of MnBiTe by Scanning Tunneling Microscopy and Spectroscopy. *Nano Letters*, **2020**, 20, 3271-3277	11.5	34
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253	Effects of strain and oxygen vacancies on the ferroelectric and antiferrodistortive distortions in PbTiO3/SrTiO3 superlattice. *Physical Review B*, **2015**, 92,	3.3	33
252	Growth of atomically thick transition metal sulfide filmson graphene/6H-SiC(0001) by molecular beam epitaxy. *Nano Research*, **2018**, 11, 4722-4727	10	32
251	First-principles study of 180? domain walls in BaTiO3: Mixed Bloch-Nēl-Ising character. *Physical Review B*, **2014**, 90,	3.3	32
250	A Chemical Modification Strategy for Hydrogen Storage in Covalent Organic Frameworks. *Journal of Physical Chemistry C*, **2010**, 114, 13402-13407	3.8	32
249	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. *Nanoscale*, **2015**, 7, 13586-90	7.7	31
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247	Voltage-controllable colossal magnetocrystalline anisotropy in single-layer transition metal dichalcogenides. *Physical Review B*, **2017**, 96,	3.3	31

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244	Field emission in doped nanotubes. *Journal of Nanoscience and Nanotechnology*, **2005**, 5, 1421-34	1.3	31
243	Elastic Properties and Fracture Behaviors of Biaxially Deformed, Polymorphic MoTe. *Nano Letters*, **2019**, 19, 761-769	11.5	31
242	Type-II Ising Superconductivity in Two-Dimensional Materials with Spin-Orbit Coupling. *Physical Review Letters*, **2019**, 123, 126402	7.4	30
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214	Magnetic anisotropy of the two-dimensional ferromagnetic insulator MnBi2Te4. *Physical Review B*, **2019**, 100,	3.3	24
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