Gang Wu

List of Publications by Year
in descending order

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71 papers	1,708 citations	279798 23 h-index	289244 40 g-index
71 all docs	71 docs citations	71 times ranked	2368 citing authors

#	Article	IF	Citations
1	A Dual-Surface Mechanism of Oxidant-Free Pyrrole Polymerization in the Two-Dimensional Titanium Carbide (MXene) Interlayer Nanospace. Journal of Physical Chemistry C, 2022, 126, 1316-1325.	3.1	5
2	Molecular simulation of linear octacosane via a CG10 coarse grain scheme. Physical Chemistry Chemical Physics, 2022, 24, 5351-5359.	2.8	1
3	Wax Inhibition by Ethylene-Vinyl Acetate Using United Atom Molecular Simulations. Energy & Fuels, 2022, 36, 861-870.	5.1	1
4	Gallium-Doped Zinc Oxide Nanostructures for Tunable Transparent Thermoelectric Films. ACS Applied Nano Materials, 2022, 5, 8631-8639.	5.0	13
5	Unravelling the Molecular Origin of Organic Semiconductors with Highâ€Performance Thermoelectric Response. Advanced Functional Materials, 2021, 31, 2007438.	14.9	14
6	Electronic transport descriptors for the rapid screening of thermoelectric materials. Materials Horizons, 2021, 8, 2463-2474.	12.2	16
7	Ab initio dipolar electron-phonon interactions in two-dimensional materials. Physical Review B, 2021, 103, .	3.2	12
8	Designing Intrinsic Topological Insulators in Two-Dimensional Metalâ€“Organic Frameworks. Journal of Physical Chemistry Letters, 2021, 12, 6934-6940.	4.6	6
9	A molecular roadmap towards organic donor-acceptor complexes with high-performance thermoelectric response. Npj Computational Materials, 2021, 7, .	8.7	12
10	Geometry and Greatly Enhanced Thermoelectric Performance of Monolayer MXY Transitionâ€Metal Dichalcogenide: MoSTe as an Example. Physica Status Solidi - Rapid Research Letters, 2021, 15, 2100166.	2.4	5
11	Molecular dynamics simulation of octacosane for phase diagrams and properties via the united-atom scheme. Physical Chemistry Chemical Physics, 2021, 23, 21262-21271.	2.8	8
12	High Spin Pro-Quinoid Benzo[1,2-c;4,5-câ€²]bisthiadiazole Conjugated Polymers for High-Performance Solution-Processable Polymer Thermoelectrics. , 2020, 2, 147-152.		43
13	Theoretical search for high-performance thermoelectric donorâ€“acceptor copolymers: the role of super-exchange couplings. Journal of Materials Chemistry A, 2020, 8, 21852-21861.	10.3	22
14	Strain Effects on the n-Type Thermoelectric Performance of the Small-Molecule Organic Semiconductor 2-5-Difluoro-7,7,8,8-Tetracyanoquinodimethane. ACS Applied Energy Materials, 2020, 3, 10174-10182.	5.1	4
15	High performance photocatalytic and thermoelectric two-dimensional asymmetrically ordered Janus-like MXene alloys. Materials Advances, 2020, 1, 1176-1185.	5.4	14
16	Effect of substituents in sulfoxides on the enhancement of thermoelectric properties of PEDOT:PSS: experimental and modelling evidence. Molecular Systems Design and Engineering, 2020, 5, 976-984.	3.4	29
17	Uniaxial negative thermal expansion and band renormalization in monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>T</mml:mi><mml:mi>d</mml:mi></mml:msub><mml:m mathvariant="normal">MoTe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> at low temperature. Physical Review B, 2020, 101, .	3.2	12
18	Conducting Polymers: The Role of Electrostatic Interaction between Free Charge Carriers and Counterions in Thermoelectric Power Factor of Conducting Polymers: From Crystalline to Polycrystalline Domains (Adv. Theory Simul. 6/2020). Advanced Theory and Simulations, 2020, 3, 2070016.	2.8	1

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19	Beyond the Mahanâ€“Sofo best thermoelectric strategy: high thermoelectric performance from directional Ï€-conjugation in two-dimensional poly(tetrathienoanthracene). Journal of Materials Chemistry A, 2020, 8, 4257-4262.	10.3	13
20	The Role of Electrostatic Interaction between Free Charge Carriers and Counterions in Thermoelectric Power Factor of Conducting Polymers: From Crystalline to Polycrystalline Domains. Advanced Theory and Simulations, 2020, 3, 2000015.	2.8	10
21	Correlating charge and thermoelectric transport to paracrystallinity in conducting polymers. Nature Communications, 2020, 11, 1737.	12.8	45
22	EPIC STAR: a reliable and efficient approach for phonon- and impurity-limited charge transport calculations. Npj Computational Materials, 2020, 6, .	8.7	31
23	Orbital-adapted electronic structure and anisotropic transport in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î³</mml:mi><mml:mtext>â^'</mml:mtext><mml:msub><mml:mi>SrTiO</mml:mi> Completely polarized <mml:math Materials, 2020, 4, .	2.4	0
24	orbitals realized in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mi>d</mml:mi><mml:mn>7</mml:mn></mml:msup><mml:m mathvariant="normal">Ni</mml:mi><mml:mrow><mml:mn>3</mml:mn><mml:mo>+</mml:mo></mml:mrow></mml:msup></mml:mat based heterointerface. Physical Review Materials, 2020, 4, .	2.4	2
25	Topological evolution of correlated band structures and heavy-fermion-like behavior in a molybdenum-based metal organic framework C48S36Mo6. Journal of Physics Condensed Matter, 2020, 32, 295503.	1.8	0
26	Unprecedented Enhancement of Thermoelectric Power Factor Induced by Pressure in Smallâ€Molecule Organic Semiconductors. Advanced Materials, 2019, 31, e1901956.	21.0	30
27	NIR light manipulated â€œpaper artâ€•for customizing devices with sophisticated structure from DA-epoxy/graphene composites. Composites Part B: Engineering, 2019, 177, 107369.	12.0	6
28	Improved Alignment of PEDOT:PSS Induced by in-situ Crystallization of â€œGreenâ€•Dimethylsulfone Molecules to Enhance the Polymer Thermoelectric Performance. Frontiers in Chemistry, 2019, 7, 783.	3.6	36
29	Self-Organization of PEDOT:PSS Induced by Green and Water-Soluble Organic Molecules. Journal of Physical Chemistry C, 2019, 123, 9745-9755.	3.1	32
30	2D Singleâ€Layer Ï€â€Conjugated Nickel Bis(dithiolene) Complex: A Goodâ€Electronâ€Poorâ€Phonon Thermoelectric Material. Advanced Electronic Materials, 2019, 5, 1800892.	5.1	21
31	A theoretical mechanistic study on electrical conductivity enhancement of DMSO treated PEDOT:PSS. Journal of Materials Chemistry C, 2018, 6, 5122-5131.	5.5	100
32	Poly(nickel-ethylenetetrathiolate) and Its Analogs: Theoretical Prediction of High-Performance Doping-Free Thermoelectric Polymers. Journal of the American Chemical Society, 2018, 140, 13200-13204.	13.7	39
33	Orbital-Engineering-Based Screening of Ï€-Conjugated d⁸ Transition-Metal Coordination Polymers for High-Performance n-Type Thermoelectric Applications. ACS Applied Materials & Interfaces, 2018, 10, 35306-35315.	8.0	32
34	Tuning the thermoelectric performance of Ï€â€“d conjugated nickel coordination polymers through metalâ€“ligand frontier molecular orbital alignment. Journal of Materials Chemistry A, 2018, 6, 19757-19766.	10.3	26
35	Pressure-induced superconductivity in MoP. Npj Quantum Materials, 2018, 3, .	5.2	32
36	Origin of metallicity in 2D multilayer nickel bis(dithiolene) sheets. 2D Materials, 2018, 5, 035027.	4.4	5

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37	Theoretical study on the self-assembly of 1,3,5-triethynylbenzene on Si(100)2 Ã— 1 and in situ polymerization via reaction with CO to fabricate a single surface-grafted polymer. Journal of Materials Chemistry C, 2017, 5, 3585-3591.	5.5	6
38	Photothermal Conversion Triggered Precisely Targeted Healing of Epoxy Resin Based on Thermoreversible Dielsâ€“Alder Network and Amino-Functionalized Carbon Nanotubes. ACS Applied Materials & Interfaces, 2017, 9, 20797-20807.	8.0	95
39	Correlation corrected phonon vibration in YTiO 3 and its effect on electronic properties. Europhysics Letters, 2017, 117, 27004.	2.0	2
40	How to Fabricate a Surface-Grafted Polythiophene on H-Si(100)2Ã—1 Surface via Self-Assembling and in Situ Surface Polymerization: A Theoretical Guide. Journal of Physical Chemistry C, 2016, 120, 25612-25619.	3.1	3
41	Several magnetic semiconductors based on the quaternary Heusler compounds. , 2015, , .		0
42	A theoretical guide for fabricating a conductive molecular wire on a silicon surface via an in situ surface polymerization reaction. Nanoscale, 2015, 7, 15277-15283.	5.6	4
43	Topological insulators based on 2D shape-persistent organic ligand complexes. Nanoscale, 2015, 7, 727-735.	5.6	46
44	Adsorption and Diffusion of CO₂ and CH₄ in Zeolitic Imidazolate Framework-8: Effect of Structural Flexibility. Journal of Physical Chemistry C, 2014, 118, 8788-8794.	3.1	132
45	A Versatile Approach towards Multifunctional Robust Microcapsules with Tunable, Restorable, and Solventâ€Proof Superhydrophobicity for Selfâ€Healing and Selfâ€Cleaning Coatings. Advanced Functional Materials, 2014, 24, 6751-6761.	14.9	129
46	First-principles study of perpendicular magnetic anisotropy in CoFe/MgO and CoFe/Mg<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>B<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:	3.2	37
47	First-principles calculations of the magnetic anisotropic constants of Coâ€“Pd multilayers: Effect of stacking faults. Europhysics Letters, 2012, 99, 17001.	2.0	6
48	Electromechanical coupling in coaxial semiconductor carbon nanotube intramolecular junctions. Europhysics Letters, 2011, 95, 37001.	2.0	0
49	Doping-Enhanced Lithium Diffusion in Lithium-Ion Batteries. Physical Review Letters, 2011, 107, 118302.	7.8	7
50	Phononics: A New Science and Technology of Controlling Heat Flow and Processing Information by Phonons. , 2010, , .		2
51	Density-gradient-corrected embedded atom method. Physical Review B, 2009, 79, .	3.2	9
52	Anomalous Heat Conduction, Diffusion and Heat Rectification in Nanoscale Structures. , 2009, , .		0
53	Structural and vibrational properties of deformed carbon nanotubes. Frontiers of Physics in China, 2009, 4, 280-296.	1.0	3
54	Itinerant Flat-Band Magnetism in Hydrogenated Carbon Nanotubes. ACS Nano, 2009, 3, 1646-1650.	14.6	17

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55	G-band Variation of Individual Single-Walled Carbon Nanotubes under Torsional Strain. Journal of Physical Chemistry C, 2008, 112, 10789-10793.	3.1	12
56	Thermal rectifiers from deformed carbon nanohorns. Journal of Physics Condensed Matter, 2008, 20, 175211.	1.8	58
57	The study of structural, electronic and optical properties of double-walled carbon nanotube bundles under hydrostatic pressure. Europhysics Letters, 2008, 81, 47003.	2.0	6
58	Thermal rectification in carbon nanotube intramolecular junctions: Molecular dynamics calculations. Physical Review B, 2007, 76, .	3.2	222
59	Raman characteristic peaks induced by the topological defects of carbon nanotube intramolecular junctions. Physical Review B, 2006, 73, .	3.2	34
60	Radial breathinglike mode of the collapsed single-walled carbon nanotube bundle under hydrostatic pressure. Applied Physics Letters, 2006, 88, 223114.	3.3	7
61	Single-walled carbon nanotube bundle under hydrostatic pressure studied by first-principles calculations. Physical Review B, 2006, 73, .	3.2	26
62	Nonlinear optical susceptibility of deformed achiral carbon nanotubes studied from first-principles calculations. Applied Physics Letters, 2006, 89, 013102.	3.3	6
63	Structural transformations of double-walled carbon nanotube bundle under hydrostatic pressure. Applied Physics Letters, 2006, 89, 113101.	3.3	41
64	Anomalous heat conduction in a carbon nanowire: Molecular dynamics calculations. Physical Review B, 2005, 71, .	3.2	28
65	Raman modes of the deformed single-wall carbon nanotubes. Physical Review B, 2005, 72, .	3.2	51
66	Radial-breathing-like phonon modes of double-walled carbon nanotubes. Physical Review B, 2005, 72, .	3.2	8
67	Linear optical properties of deformed carbon nanotubes. Physical Review B, 2004, 70, .	3.2	16
68	Heat conduction in a carbon chain. Physics Letters, Section A: General, Atomic and Solid State Physics, 2004, 325, 403-406.	2.1	9
69	Noise-induced order phenomenon in semiquantum system. Physics Letters, Section A: General, Atomic and Solid State Physics, 2003, 308, 391-396.	2.1	0
70	Control of Semiquantum Chaos by the Nonfeedback Method. Chinese Physics Letters, 2002, 19, 1763-1766.	3.3	2
71	Characteristics of the wave function of coupled oscillators in semiquantum chaos. Physics Letters, Section A: General, Atomic and Solid State Physics, 2002, 300, 199-204.	2.1	0