

Sheng Meng

List of Publications by Year in descending order

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298
papers

15,549
citations

18436

62
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21474

114
g-index

302
all docs

302
docs citations

302
times ranked

16691
citing authors

#	ARTICLE	IF	CITATIONS
1	Experimental realization of two-dimensional boron sheets. Nature Chemistry, 2016, 8, 563-568.	6.6	1,398
2	Evidence of Silicene in Honeycomb Structures of Silicon on Ag(111). Nano Letters, 2012, 12, 3507-3511.	4.5	1,190
3	Evidence for Dirac Fermions in a Honeycomb Lattice Based on Silicon. Physical Review Letters, 2012, 109, 056804.	2.9	634
4	Water adsorption on metal surfaces: A general picture from density functional theory studies. Physical Review B, 2004, 69, .	1.1	448
5	Graphene NanoFlakes with Large Spin. Nano Letters, 2008, 8, 241-245.	4.5	443
6	Adsorption and Diffusion of Lithium on Layered Silicon for Li-Ion Storage. Nano Letters, 2013, 13, 2258-2263.	4.5	377
7	Dirac Fermions in Borophene. Physical Review Letters, 2017, 118, 096401.	2.9	353
8	Topological Frustration in Graphene Nanoflakes: Magnetic Order and Spin Logic Devices. Physical Review Letters, 2009, 102, 157201.	2.9	237
9	Vibrational Recognition of Hydrogen-Bonded Water Networks on a Metal Surface. Physical Review Letters, 2002, 89, 176104.	2.9	229
10	Spontaneous Symmetry Breaking and Dynamic Phase Transition in Monolayer Silicene. Physical Review Letters, 2013, 110, 085504.	2.9	205
11	Natural Dyes Adsorbed on TiO_2 Nanowire for Photovoltaic Applications: Enhanced Light Absorption and Ultrafast Electron Injection. Nano Letters, 2008, 8, 3266-3272.	4.5	198
12	Real-time, local basis-set implementation of time-dependent density functional theory for excited state dynamics simulations. Journal of Chemical Physics, 2008, 129, 054110.	1.2	191
13	Structural Model of Eumelanin. Physical Review Letters, 2006, 97, 218102.	2.9	170
14	Towards understanding the effects of carbon and nitrogen-doped carbon coating on the electrochemical performance of $\text{Li}_4\text{Ti}_5\text{O}_{12}$ in lithium ion batteries: a combined experimental and theoretical study. Physical Chemistry Chemical Physics, 2011, 13, 15127.	1.3	169
15	First Principles Design of Dye Molecules with Ullazine Donor for Dye Sensitized Solar Cells. Journal of Physical Chemistry C, 2013, 117, 3772-3778.	1.5	169
16	DNA Nucleoside Interaction and Identification with Carbon Nanotubes. Nano Letters, 2007, 7, 45-50.	4.5	156
17	Direct evidence of metallic bands in a monolayer boron sheet. Physical Review B, 2016, 94, .	1.1	152
18	Electron and Hole Dynamics in Dye-Sensitized Solar Cells: Influencing Factors and Systematic Trends. Nano Letters, 2010, 10, 1238-1247.	4.5	137

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19	Emergence of electron coherence and two-color all-optical switching in MoS ₂ based on spatial self-phase modulation. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 11800-11805.	3.3	133
20	Complexation of Flavonoids with Iron: Structure and Optical Signatures. Journal of Physical Chemistry B, 2008, 112, 1845-1850.	1.2	132
21	Robust Stacking-Independent Ultrafast Charge Transfer in MoS ₂ /WS ₂ Bilayers. ACS Nano, 2017, 11, 12020-12026.	7.3	130
22	Interfacial Oxygen Vacancies as a Potential Cause of Hysteresis in Perovskite Solar Cells. Chemistry of Materials, 2016, 28, 802-812.	3.2	128
23	Monitoring Local Strain Vector in Atomic-Layered MoSe ₂ by Second-Harmonic Generation. Nano Letters, 2017, 17, 7539-7543.	4.5	128
24	Ordered and Reversible Hydrogenation of Silicene. Physical Review Letters, 2015, 114, 126101.	2.9	127
25	Correlations between Immobilizing Ions and Suppressing Hysteresis in Perovskite Solar Cells. ACS Energy Letters, 2016, 1, 266-272.	8.8	118
26	Metal-Diboride Nanotubes as High-Capacity Hydrogen Storage Media. Nano Letters, 2007, 7, 663-667.	4.5	115
27	Predicting Energy Conversion Efficiency of Dye Solar Cells from First Principles. Journal of Physical Chemistry C, 2014, 118, 16447-16457.	1.5	115
28	Quantized Water Transport: Ideal Desalination through Graphyne-4 Membrane. Scientific Reports, 2013, 3, 3163.	1.6	113
29	Quantum Mode Selectivity of Plasmon-Induced Water Splitting on Gold Nanoparticles. ACS Nano, 2016, 10, 5452-5458.	7.3	106
30	pH-Dependent Synthesis of Novel Structure-Controllable Polymer-Carbon NanoDots with High Acidophilic Luminescence and Super Carbon Dots Assembly for White Light-Emitting Diodes. ACS Applied Materials & Interfaces, 2016, 8, 4062-4068.	4.0	106
31	Water adsorption on hydroxylated silica surfaces studied using the density functional theory. Physical Review B, 2005, 71, .	1.1	105
32	A Resistance-Switchable and Ferroelectric Metal-Organic Framework. Journal of the American Chemical Society, 2014, 136, 17477-17483.	6.6	103
33	Theoretical Models of Eumelanin Protomolecules and their Optical Properties. Biophysical Journal, 2008, 94, 2095-2105.	0.2	100
34	Laser picoscopy of valence electrons in solids. Nature, 2020, 583, 55-59.	13.7	100
35	First-principles study of water on copper and noble metal (110) surfaces. Physical Review B, 2008, 77, .	1.1	99
36	Solution-Processable, Low-Voltage, and High-Performance Monolayer Field-Effect Transistors with Aqueous Stability and High Sensitivity. Advanced Materials, 2015, 27, 2113-2120.	11.1	97

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37	From Silicene to Half-Silicane by Hydrogenation. ACS Nano, 2015, 9, 11192-11199.	7.3	97
38	Side-group chemical gating via reversible optical and electric control in a single molecule transistor. Nature Communications, 2019, 10, 1450.	5.8	96
39	Interface-Engineered Plasmonics in Metal/Semiconductor Heterostructures. Advanced Energy Materials, 2016, 6, 1600431.	10.2	95
40	A new phase diagram of water under negative pressure: The rise of the lowest-density clathrate s-III. Science Advances, 2016, 2, e1501010.	4.7	92
41	Design of a Photoactive Hybrid Bilayer Dielectric for Flexible Nonvolatile Organic Memory Transistors. ACS Nano, 2016, 10, 436-445.	7.3	91
42	Discovery of 2D Anisotropic Dirac Cones. Advanced Materials, 2018, 30, 1704025.	11.1	91
43	Atomic Structure and Bonding of Water Overlayer on Cu(110): The Borderline for Intact and Dissociative Adsorption. Journal of the American Chemical Society, 2006, 128, 9282-9283.	6.6	90
44	Suppressed superconductivity in substrate-supported Bi_2Te_3 borophene by tensile strain and electron doping. 2D Materials, 2017, 4, 025032.	2.0	90
45	Observation of Dirac Cone Warping and Chirality Effects in Silicene. ACS Nano, 2013, 7, 9049-9054.	7.3	88
46	Ice Tessellation on a Hydroxylated Silica Surface. Physical Review Letters, 2004, 92, 146102.	2.9	87
47	Characterizing hydrophobicity of amino acid side chains in a protein environment via measuring contact angle of a water nanodroplet on planar peptide network. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 12946-12951.	3.3	87
48	Interlayer-State-Coupling Dependent Ultrafast Charge Transfer in MoS_2/WS_2 Bilayers. Advanced Science, 2017, 4, 1700086.	5.6	87
49	Photoinduced Nonequilibrium Topological States in Strained Black Phosphorus. Physical Review Letters, 2018, 120, 237403.	2.9	80
50	Design of Dye Acceptors for Photovoltaics from First-Principles Calculations. Journal of Physical Chemistry C, 2011, 115, 9276-9282.	1.5	78
51	Metastable phases of 2D boron sheets on $\text{Ag}(1\bar{1}0)$. Journal of Physics Condensed Matter, 2017, 29, 095002.	0.7	78
52	Properties of copper (fluoro-)phthalocyanine layers deposited on epitaxial graphene. Journal of Chemical Physics, 2011, 134, 194706.	1.2	77
53	Comment on Graphene Nanoflakes with Large Spin: A Broken-Symmetry States. Nano Letters, 2008, 8, 766-766.	4.5	76
54	Water printing of ferroelectric polarization. Nature Communications, 2018, 9, 3809.	5.8	75

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55	The Origin of Oxygen Vacancies Controlling La _{2/3} Sr _{1/3} MnO ₃ Electronic and Magnetic Properties. <i>Advanced Materials Interfaces</i> , 2016, 3, 1500753.	1.9	73
56	Intrinsic valley polarization of magnetic VSe ₂ monolayers. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 255501.	0.7	73
57	Influence of water on the electronic structure of metal-supported graphene: Insights from van der Waals density functional theory. <i>Physical Review B</i> , 2012, 85, .	1.1	70
58	Stacking-dependent electronic structure of bilayer silicene. <i>Applied Physics Letters</i> , 2014, 104, .	1.5	70
59	Atomic Disorders Induced by Silver and Magnesium Ion Migrations Favor High Thermoelectric Performance in \pm MgAgSb-Based Materials. <i>Advanced Functional Materials</i> , 2015, 25, 6478-6488.	7.8	70
60	Structure-Property Relations in All-Organic Dye-Sensitized Solar Cells. <i>Advanced Functional Materials</i> , 2013, 23, 424-429.	7.8	68
61	Microscopic Insight into Surface Wetting: Relations between Interfacial Water Structure and the Underlying Lattice Constant. <i>Physical Review Letters</i> , 2013, 110, 126101.	2.9	67
62	Integrated Plasmonics: Broadband Dirac Plasmons in Borophene. <i>Physical Review Letters</i> , 2020, 125, 116802.	2.9	67
63	Photoexcitation in Solids: First-Principles Quantum Simulations by Real-Time TDDFT. <i>Advanced Theory and Simulations</i> , 2018, 1, 1800055.	1.3	64
64	Field and temperature dependence of intrinsic diamagnetism in graphene: Theory and experiment. <i>Physical Review B</i> , 2015, 91, .	1.1	61
65	Determination of DNA-Base Orientation on Carbon Nanotubes through Directional Optical Absorbance. <i>Nano Letters</i> , 2007, 7, 2312-2316.	4.5	60
66	Nonlinear Rashba spin splitting in transition metal dichalcogenide monolayers. <i>Nanoscale</i> , 2016, 8, 17854-17860.	2.8	60
67	A molecular picture of hydrophilic and hydrophobic interactions from ab initio density functional theory calculations. <i>Journal of Chemical Physics</i> , 2003, 119, 7617-7620.	1.2	59
68	Consistent picture for the wetting structure of water/Ru(0001). <i>Chemical Physics Letters</i> , 2005, 402, 384-388.	1.2	57
69	Flexible strain sensors with high performance based on metallic glass thin film. <i>Applied Physics Letters</i> , 2017, 111, .	1.5	55
70	The 2021 ultrafast spectroscopic probes of condensed matter roadmap. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 353001.	0.7	55
71	Screening Magnetic Two-Dimensional Atomic Crystals with Nontrivial Electronic Topology. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 6709-6715.	2.1	53
72	Ultrafast charge ordering by self-amplified exciton-phonon dynamics in TiSe ₂ . <i>Nature Communications</i> , 2020, 11, 43.	5.8	53

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73	First-principles studies of cation-doped spinel LiMn_2O_4 for lithium ion batteries. <i>Physical Review B</i> , 2003, 67, .	1.1	51
74	Cooperativity in Surface Bonding and Hydrogen Bonding of Water and Hydroxyl at Metal Surfaces. <i>Journal of Physical Chemistry C</i> , 2010, 114, 10240-10248.	1.5	51
75	Novel Excitonic Solar Cells in Phosphorene TiO_2 Heterostructures with Extraordinary Charge Separation Efficiency. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1880-1887.	2.1	51
76	Transparent proton transport through a two-dimensional nanomesh material. <i>Nature Communications</i> , 2019, 10, 3971.	5.8	50
77	Giant enhancement of optical nonlinearity in two-dimensional materials by multiphoton-excitation resonance energy transfer from quantum dots. <i>Nature Photonics</i> , 2021, 15, 510-515.	15.6	50
78	New Pathway for Hot Electron Relaxation in Two-Dimensional Heterostructures. <i>Nano Letters</i> , 2018, 18, 6057-6063.	4.5	49
79	Transport behavior of water molecules through two-dimensional nanopores. <i>Journal of Chemical Physics</i> , 2014, 141, 18C528.	1.2	48
80	Controlling Adsorption Structure of Eosin Y Dye on Nanocrystalline TiO_2 Films for Improved Photovoltaic Performances. <i>Journal of Physical Chemistry C</i> , 2013, 117, 14659-14666.	1.5	47
81	Ideal type-II Weyl phonons in wurtzite CuI . <i>Physical Review B</i> , 2019, 100, .	1.1	45
82	Water adsorption on a NaCl (001) surface: A density functional theory study. <i>Physical Review B</i> , 2006, 74, .	1.1	43
83	D- π -A Dye System Containing Cyano-Benzoic Acid as Anchoring Group for Dye-Sensitized Solar Cells. <i>Langmuir</i> , 2011, 27, 14248-14252.	1.6	41
84	Modeling charge recombination in dye-sensitized solar cells using first-principles electron dynamics: effects of structural modification. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 17187.	1.3	41
85	Theoretical Insights into Ultrafast Dynamics in Quantum Materials. <i>Ultrafast Science</i> , 2022, 2022, .	5.8	40
86	Mechanisms for Ultrafast Nonradiative Relaxation in Electronically Excited Eumelanin Constituents. <i>Biophysical Journal</i> , 2008, 95, 4396-4402.	0.2	39
87	The effect of moiré superstructures on topological edge states in twisted bismuthene homojunctions. <i>Science Advances</i> , 2020, 6, eaba2773.	4.7	39
88	Controlling states of water droplets on nanostructured surfaces by design. <i>Nanoscale</i> , 2017, 9, 18240-18245.	2.8	38
89	Dual-gated single-molecule field-effect transistors beyond Moore's law. <i>Nature Communications</i> , 2022, 13, 1410.	5.8	38
90	Selective adsorption and electronic interaction of F16CuPc on epitaxial graphene. <i>Physical Review B</i> , 2010, 82, .	1.1	37

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91	Superconductivity in dense carbon-based materials. <i>Physical Review B</i> , 2016, 93, .	1.1	37
92	Plasmon-Induced Ultrafast Hydrogen Production in Liquid Water. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 63-69.	2.1	37
93	Probing Nonequilibrium Dynamics of Photoexcited Polarons on a Metal-Oxide Surface with Atomic Precision. <i>Physical Review Letters</i> , 2020, 124, 206801.	2.9	37
94	Observation of Topological Flat Bands in the Kagome Semiconductor Nb ₃ Cl ₈ . <i>Nano Letters</i> , 2022, 22, 4596-4602.	4.5	37
95	Tuning Solid Surfaces from Hydrophobic to Superhydrophilic by Submonolayer Surface Modification. <i>Physical Review Letters</i> , 2006, 97, 036107.	2.9	36
96	Benign Interfacial Iodine Vacancies in Perovskite Solar Cells. <i>Journal of Physical Chemistry C</i> , 2017, 121, 5905-5913.	1.5	36
97	Quartic anharmonicity and anomalous thermal conductivity in cubic antiperovskites $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{A} \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 3 \langle \text{mml:mn} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \text{mathvariant="normal"} \rangle \text{O} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle \langle \text{mml:math} \rangle$		

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109	<i>Ab initio</i> evidence for nonthermal characteristics in ultrafast laser melting. <i>Physical Review B</i> , 2016, 94, .	1.1	32
110	Three-dimensional metal-intercalated covalent organic frameworks for near-ambient energy storage. <i>Scientific Reports</i> , 2013, 3, 1882.	1.6	31
111	Photoexcitation Induced Quantum Dynamics of Charge Density Wave and Emergence of a Collective Mode in TaS_2 . <i>Nano Letters</i> , 2019, 19, 6027-6034.	4.5	31
112	Ultrafast Optical Modulation of Harmonic Generation in Two-Dimensional Materials. <i>Nano Letters</i> , 2020, 20, 8053-8058.	4.5	31
113	Reversible Transition between Thermodynamically Stable Phases with Low Density of Oxygen Vacancies on the $SrTiO_3$ surface. <i>ACS Nano</i> , 2019, 13, 10000-10007.	2.9	30
114	Turning on and off the Rotational Oscillation of a Single Porphine Molecule by Molecular Charge State. <i>ACS Nano</i> , 2012, 6, 4132-4136.	7.3	30
115	Chen <i>et al.</i> Reply. <i>Physical Review Letters</i> , 2013, 110, 229702.	2.9	30
116	Plasmon-induced dynamics of H ₂ splitting on a silver atomic chain. <i>Applied Physics Letters</i> , 2015, 107, .	1.5	30
117	Dissolution dynamics of NaCl nanocrystal in liquid water. <i>Physical Review E</i> , 2005, 72, 012602.	0.8	29
118	Quantum plasmonics: Symmetry-dependent plasmon-molecule coupling and quantized photoconductances. <i>Physical Review B</i> , 2012, 86, .	1.1	29
119	Photocontrol of charge injection/extraction at electrode/semiconductor interfaces for high-photoresponsivity organic transistors. <i>Journal of Materials Chemistry C</i> , 2016, 4, 5289-5296.	2.7	29
120	Plasmon-driven sub-picosecond breathing of metal nanoparticles. <i>Nanoscale</i> , 2017, 9, 12391-12397.	2.8	29
121	Ultrafast Broadband Charge Collection from Clean Graphene/CH ₃ NH ₃ PbI ₃ Interface. <i>Journal of the American Chemical Society</i> , 2018, 140, 14952-14957.	6.6	29
122	Electronic Structures and Catalytic Activities of Niobium Oxides as Electrocatalysts in Liquid Junction Photovoltaic Devices. <i>Solar Rrl</i> , 2020, 4, 1900430.	3.1	29
123	Optical Control of Multistage Phase Transition via Phonon Coupling in $MoTe_2$. <i>Physical Review Letters</i> , 2022, 128, 015702.	2.9	29
124	Multilayered silicene: the bottom-up approach for a weakly relaxed Si(111) with Dirac surface states. <i>Nanoscale</i> , 2015, 7, 15880-15885.	2.8	28
125	Recent progresses in real-time local-basis implementation of time dependent density functional theory for electron-nucleus dynamics. <i>Computational Materials Science</i> , 2016, 112, 478-486.	1.4	28
126	Two-gap and three-gap superconductivity in AlB_2 -based films. <i>Physical Review B</i> , 2019, 100, .	1.4	28

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127	Spin-Orientation-Dependent Topological States in Two-Dimensional Antiferromagnetic NiTe ₂ S ₄ Monolayers. Nano Letters, 2019, 19, 3321-3326.	4.5	28
128	Flat AgTe Honeycomb Monolayer on Ag(111). Journal of Physical Chemistry Letters, 2019, 10, 1866-1871.	2.1	28
129	Effective Hamiltonian for FeAs-based superconductors. Physical Review B, 2008, 78, .	1.1	27
130	Basic science of water: Challenges and current status towards a molecular picture. Nano Research, 2015, 8, 3085-3110.	5.8	27
131	Wetting behavior of water on silicon carbide polar surfaces. Physical Chemistry Chemical Physics, 2016, 18, 28033-28039.	1.3	27
132	Structure and quantum well states in silicene nanoribbons on Ag(110). Surface Science, 2016, 645, 74-79.	0.8	27
133	Atomistic nature of NaCl nucleation at the solid-liquid interface. Journal of Chemical Physics, 2007, 126, 044708.	1.2	26
134	High thermopower and potential thermoelectric properties of crystalline LiH and NaH. Physical Review B, 2017, 95, .	1.1	26
135	Superstructure-Induced Splitting of Dirac Cones in Silicene. Physical Review Letters, 2019, 122, 196801.	2.9	26
136	Two-dimensional hydration shells of alkali metal ions at a hydrophobic surface. Journal of Chemical Physics, 2004, 121, 12572.	1.2	25
137	Exotic thermoelectric behavior in nitrogenated holey graphene. RSC Advances, 2017, 7, 25803-25810.	1.7	25
138	Effects of line defects on the electronic and optical properties of strain-engineered WO ₃ thin films. Journal of Materials Chemistry C, 2017, 5, 11694-11699.	2.7	25
139	Universal Scaling of Intrinsic Resistivity in Two-Dimensional Metallic Borophene. Angewandte Chemie - International Edition, 2018, 57, 4585-4589.	7.2	25
140	Hidden spin polarization in the 1 T -phase layered transition-metal dichalcogenides MX ₂ (M = Zr, Hf; X = S, Se, Te). Physical Review Letters, 2019, 122, 196801.	4.8	25
141	Identifying Few-Molecule Water Clusters with High Precision on Au(111) Surface. ACS Nano, 2018, 12, 6452-6457.	7.3	25
142	Water transport through subnanopores in the ultimate size limit: Mechanism from molecular dynamics. Nano Research, 2019, 12, 587-592.	5.8	25
143	Manipulating Weyl quasiparticles by orbital-selective photoexcitation in WTe ₂ . Nature Communications, 2021, 12, 1885.	5.8	25
144	Cooperative evolution of intraband and interband excitations for high-harmonic generation in strained MoS ₂ . Physical Review B, 2019, 99, .	1.1	24

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145	Anomalous electronic and thermoelectric transport properties in cubic RbMn_2Sb antiperovskite. <i>Physical Review B</i> , 2020, 102, .	1.3	24
146	Indirect to Direct Charge Transfer Transition in Plasmon-Enabled CO_2 Photoreduction. <i>Advanced Science</i> , 2022, 9, e2102978.	5.6	24
147	Intrinsic electronic transport and thermoelectric power factor in n-type doped monolayer MoS_2 . <i>New Journal of Physics</i> , 2018, 20, 043009.	1.2	23
148	Phonon thermal transport in a class of graphene allotropes from first principles. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 15980-15985.	1.3	23
149	Screening two-dimensional materials with topological flat bands. <i>Physical Review Materials</i> , 2021, 5, .	0.9	23
150	Prediction of two-dimensional electron gas mediated magnetoelectric coupling at ferroelectric PbTiO_3 heterostructures. <i>Physical Review B</i> , 2017, 95, .	1.1	22
151	Nonadiabatic Dynamics of Photocatalytic Water Splitting on A Polymeric Semiconductor. <i>Nano Letters</i> , 2021, 21, 6449-6455.	4.5	22
152	Menget al.Reply:. <i>Physical Review Letters</i> , 2003, 91, .	2.9	21
153	Momentum-resolved TDDFT algorithm in atomic basis for real time tracking of electronic excitation. <i>Journal of Chemical Physics</i> , 2018, 149, 154104.	1.2	21
154	A molecular dynamics study of hydration and dissolution of NaCl nanocrystal in liquid water. <i>Journal of Physics Condensed Matter</i> , 2006, 18, 10165-10177.	0.7	20
155	Water wettability of close-packed metal surfaces. <i>Journal of Chemical Physics</i> , 2007, 127, 244710.	1.2	20
156	Quinoid conjugated dye designed for efficient sensitizer in dye sensitized solar cells. <i>Chemical Physics Letters</i> , 2013, 586, 97-99.	1.2	20
157	Carbene-mediated self-assembly of diamondoids on metal surfaces. <i>Nanoscale</i> , 2016, 8, 8966-8975.	2.8	20
158	An Iron-Porphyrin Complex with Large Easy-Axis Magnetic Anisotropy on Metal Substrate. <i>ACS Nano</i> , 2017, 11, 11402-11408.	7.3	20
159	Dirac cone pairs in silicene induced by interface Si-Ag hybridization: A first-principles effective band study. <i>Physical Review B</i> , 2017, 95, .	1.1	20
160	Hexagonal Monolayer Ice without Shared Edges. <i>Physical Review Letters</i> , 2018, 121, 256001.	2.9	20
161	Monolayer puckered pentagonal VTe_2 : An emergent two-dimensional ferromagnetic semiconductor with multiferroic coupling. <i>Nano Research</i> , 2022, 15, 1486-1491.	5.8	20
162	Dye Sensitized Solar Cells Principles and New Design. , 0, , .		19

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163	Long-Lived Multifunctional Superhydrophobic Heterostructure Via Molecular Self-Supply. <i>Advanced Materials Interfaces</i> , 2016, 3, 1500727.	1.9	19
164	Plasmon-induced nonlinear response of silver atomic chains. <i>Nanoscale</i> , 2018, 10, 8600-8605.	2.8	19
165	Water wetting on representative metal surfaces: Improved description from van der Waals density functionals. <i>Chemical Physics Letters</i> , 2012, 521, 161-166.	1.2	18
166	Magnetic Dirac fermions and Chern insulator supported on pristine silicon surface. <i>Physical Review B</i> , 2016, 94, .	1.1	18
167	Nucleation and dissociation of methane clathrate embryo at the gas-water interface. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 23410-23415.	3.3	18
168	Fermionic Analogue of High Temperature Hawking Radiation in Black Phosphorus. <i>Chinese Physics Letters</i> , 2020, 37, 067101.	1.3	18
169	MgB_4 trilayer film: A four-gap superconductor. <i>Physical Review B</i> , 2020, 101, .	1.1	18
170	First-principles dynamics of photoexcited molecules and materials towards a quantum description. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1492.	6.2	18
171	Tunable electron-phonon coupling superconductivity in platinum diselenide. <i>Physical Review Materials</i> , 2017, 1, .	0.9	18
172	Orbital Dependence in Single-Atom Electrocatalytic Reactions. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 5969-5976.	2.1	18
173	Silicene: from monolayer to multilayer – A concise review. <i>Chinese Physics B</i> , 2015, 24, 086102.	0.7	17
174	Bis(pyrazol-1-yl)methane as Non-Chromophoric Ancillary Ligand for Charged Bis-Cyclometalated Iridium(III) Complexes. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 3209-3215.	1.0	16
175	Extreme nonlinear strong-field photoemission from carbon nanotubes. <i>Nature Communications</i> , 2019, 10, 4891.	5.8	16
176	Water nanostructure formation on oxide probed in situ by optical resonances. <i>Science Advances</i> , 2019, 5, eaax6973.	4.7	16
177	Improving Photovoltaic Stability and Performance of Perovskite Solar Cells by Molecular Interface Engineering. <i>Journal of Physical Chemistry C</i> , 2019, 123, 1219-1225.	1.5	16
178	Atomically Precise Engineering of Single-Molecule Stereoelectronic Effect. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 12274-12278.	7.2	16
179	Low lattice thermal conductivity and good thermoelectric performance of cinnabar. <i>Physical Review Materials</i> , 2017, 1, .	0.9	16
180	Ultrafast Internal Exciton Dissociation through Edge States in MoS_2 Nanosheets with Diffusion Blocking. <i>Nano Letters</i> , 2022, 22, 5651-5658.	4.5	16

#	ARTICLE	IF	CITATIONS
181	Optical properties of clusters and molecules from real-time time-dependent density functional theory using a self-consistent field. <i>Molecular Physics</i> , 2010, 108, 1829-1844.	0.8	15
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