

# Sheng Meng

## List of Publications by Citations

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284  
papers

11,919  
citations

56  
h-index

101  
g-index

302  
ext. papers

13,691  
ext. citations

7  
avg, IF

6.58  
L-index

#	Paper	IF	Citations
284	Evidence of silicene in honeycomb structures of silicon on Ag(111). <i>Nano Letters</i> , <b>2012</b> , 12, 3507-11	11.5	1055
283	Experimental realization of two-dimensional boron sheets. <i>Nature Chemistry</i> , <b>2016</b> , 8, 563-8	17.6	996
282	Evidence for Dirac fermions in a honeycomb lattice based on silicon. <i>Physical Review Letters</i> , <b>2012</b> , 109, 056804	7.4	577
281	Water adsorption on metal surfaces: A general picture from density functional theory studies. <i>Physical Review B</i> , <b>2004</b> , 69,	3.3	404
280	Graphene nanoFlakes with large spin. <i>Nano Letters</i> , <b>2008</b> , 8, 241-5	11.5	393
279	Adsorption and diffusion of lithium on layered silicon for Li-ion storage. <i>Nano Letters</i> , <b>2013</b> , 13, 2258-63	11.5	299
278	Dirac Fermions in Borophene. <i>Physical Review Letters</i> , <b>2017</b> , 118, 096401	7.4	256
277	Topological frustration in graphene nanoflakes: magnetic order and spin logic devices. <i>Physical Review Letters</i> , <b>2009</b> , 102, 157201	7.4	209
276	Vibrational recognition of hydrogen-bonded water networks on a metal surface. <i>Physical Review Letters</i> , <b>2002</b> , 89, 176104	7.4	207
275	Spontaneous symmetry breaking and dynamic phase transition in monolayer silicene. <i>Physical Review Letters</i> , <b>2013</b> , 110, 085504	7.4	193
274	Natural dyes adsorbed on TiO <sub>2</sub> nanowire for photovoltaic applications: enhanced light absorption and ultrafast electron injection. <i>Nano Letters</i> , <b>2008</b> , 8, 3266-72	11.5	181
273	Towards understanding the effects of carbon and nitrogen-doped carbon coating on the electrochemical performance of Li <sub>4</sub> Ti <sub>5</sub> O <sub>12</sub> in lithium ion batteries: a combined experimental and theoretical study. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 15127-33	3.6	157
272	Real-time, local basis-set implementation of time-dependent density functional theory for excited state dynamics simulations. <i>Journal of Chemical Physics</i> , <b>2008</b> , 129, 054110	3.9	151
271	First Principles Design of Dye Molecules with Ullazine Donor for Dye Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 3772-3778	3.8	149
270	Structural model of eumelanin. <i>Physical Review Letters</i> , <b>2006</b> , 97, 218102	7.4	148
269	DNA nucleoside interaction and identification with carbon nanotubes. <i>Nano Letters</i> , <b>2007</b> , 7, 45-50	11.5	144
268	Electron and hole dynamics in dye-sensitized solar cells: influencing factors and systematic trends. <i>Nano Letters</i> , <b>2010</b> , 10, 1238-47	11.5	116

267	Direct evidence of metallic bands in a monolayer boron sheet. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	113
266	Metal-diboride nanotubes as high-capacity hydrogen storage media. <i>Nano Letters</i> , <b>2007</b> , 7, 663-7	11.5	108
265	Ordered and reversible hydrogenation of silicene. <i>Physical Review Letters</i> , <b>2015</b> , 114, 126101	7.4	106
264	Complexation of flavonoids with iron: structure and optical signatures. <i>Journal of Physical Chemistry B</i> , <b>2008</b> , 112, 1845-50	3.4	103
263	Interfacial Oxygen Vacancies as a Potential Cause of Hysteresis in Perovskite Solar Cells. <i>Chemistry of Materials</i> , <b>2016</b> , 28, 802-812	9.6	102
262	Emergence of electron coherence and two-color all-optical switching in MoS2 based on spatial self-phase modulation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2015</b> , 112, 11800-5	11.5	100
261	Quantized water transport: ideal desalination through graphyne-4 membrane. <i>Scientific Reports</i> , <b>2013</b> , 3, 3163	4.9	95
260	Water adsorption on hydroxylated silica surfaces studied using the density functional theory. <i>Physical Review B</i> , <b>2005</b> , 71,	3.3	95
259	Correlations between Immobilizing Ions and Suppressing Hysteresis in Perovskite Solar Cells. <i>ACS Energy Letters</i> , <b>2016</b> , 1, 266-272	20.1	93
258	First-principles study of water on copper and noble metal (110) surfaces. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	92
257	Predicting Energy Conversion Efficiency of Dye Solar Cells from First Principles. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 16447-16457	3.8	89
256	Robust Stacking-Independent Ultrafast Charge Transfer in MoS/WS Bilayers. <i>ACS Nano</i> , <b>2017</b> , 11, 12020-12026	10.26	89
255	pH-Dependent Synthesis of Novel Structure-Controllable Polymer-Carbon NanoDots with High Acidophilic Luminescence and Super Carbon Dots Assembly for White Light-Emitting Diodes. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2016</b> , 8, 4062-8	9.5	86
254	Theoretical models of eumelanin protomolecules and their optical properties. <i>Biophysical Journal</i> , <b>2008</b> , 94, 2095-105	2.9	86
253	Solution-processable, low-voltage, and high-performance monolayer field-effect transistors with aqueous stability and high sensitivity. <i>Advanced Materials</i> , <b>2015</b> , 27, 2113-20	24	85
252	A resistance-switchable and ferroelectric metal-organic framework. <i>Journal of the American Chemical Society</i> , <b>2014</b> , 136, 17477-83	16.4	85
251	Atomic structure and bonding of water overlayer on Cu(110): the borderline for intact and dissociative adsorption. <i>Journal of the American Chemical Society</i> , <b>2006</b> , 128, 9282-3	16.4	85
250	Observation of Dirac cone warping and chirality effects in silicene. <i>ACS Nano</i> , <b>2013</b> , 7, 9049-54	16.7	83

249	Monitoring Local Strain Vector in Atomic-Layered MoSe by Second-Harmonic Generation. <i>Nano Letters</i> , <b>2017</b> , 17, 7539-7543	11.5	80
248	Ice tessellation on a hydroxylated silica surface. <i>Physical Review Letters</i> , <b>2004</b> , 92, 146102	7.4	79
247	Quantum Mode Selectivity of Plasmon-Induced Water Splitting on Gold Nanoparticles. <i>ACS Nano</i> , <b>2016</b> , 10, 5452-8	16.7	79
246	Design of a Photoactive Hybrid Bilayer Dielectric for Flexible Nonvolatile Organic Memory Transistors. <i>ACS Nano</i> , <b>2016</b> , 10, 436-45	16.7	77
245	From Silicene to Half-Silicane by Hydrogenation. <i>ACS Nano</i> , <b>2015</b> , 9, 11192-9	16.7	76
244	A new phase diagram of water under negative pressure: The rise of the lowest-density clathrate s-III. <i>Science Advances</i> , <b>2016</b> , 2, e1501010	14.3	75
243	Properties of copper (fluoro-)phthalocyanine layers deposited on epitaxial graphene. <i>Journal of Chemical Physics</i> , <b>2011</b> , 134, 194706	3.9	75
242	Interface-Engineered Plasmonics in Metal/Semiconductor Heterostructures. <i>Advanced Energy Materials</i> , <b>2016</b> , 6, 1600431	21.8	72
241	Comment on graphene nanoflakes with large spin: broken-symmetry states. <i>Nano Letters</i> , <b>2008</b> , 8, 766	11.5	70
240	Design of Dye Acceptors for Photovoltaics from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 9276-9282	3.8	69
239	Suppressed superconductivity in substrate-supported $\sqrt{2}$ borophene by tensile strain and electron doping. <i>2D Materials</i> , <b>2017</b> , 4, 025032	5.9	63
238	Discovery of 2D Anisotropic Dirac Cones. <i>Advanced Materials</i> , <b>2018</b> , 30, 1704025	24	62
237	Interlayer-State-Coupling Dependent Ultrafast Charge Transfer in MoS/WS Bilayers. <i>Advanced Science</i> , <b>2017</b> , 4, 1700086	13.6	61
236	Atomic Disorders Induced by Silver and Magnesium Ion Migrations Favor High Thermoelectric Performance in $\sqrt{3}\sqrt{3}$ MgAgSb-Based Materials. <i>Advanced Functional Materials</i> , <b>2015</b> , 25, 6478-6488	15.6	61
235	Influence of water on the electronic structure of metal-supported graphene: Insights from van der Waals density functional theory. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	61
234	Structure-Property Relations in All-Organic Dye-Sensitized Solar Cells. <i>Advanced Functional Materials</i> , <b>2013</b> , 23, 424-429	15.6	61
233	Microscopic insight into surface wetting: relations between interfacial water structure and the underlying lattice constant. <i>Physical Review Letters</i> , <b>2013</b> , 110, 126101	7.4	58
232	The Origin of Oxygen Vacancies Controlling La <sub>2</sub> /3Sr <sub>1</sub> /3MnO <sub>3</sub> Electronic and Magnetic Properties. <i>Advanced Materials Interfaces</i> , <b>2016</b> , 3, 1500753	4.6	58

231	Metastable phases of 2D boron sheets on Ag(1 1 1). <i>Journal of Physics Condensed Matter</i> , <b>2017</b> , 29, 095002	3.8	57
230	Stacking-dependent electronic structure of bilayer silicene. <i>Applied Physics Letters</i> , <b>2014</b> , 104, 131904	3.4	57
229	Characterizing hydrophobicity of amino acid side chains in a protein environment via measuring contact angle of a water nanodroplet on planar peptide network. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2016</b> , 113, 12946-12951	11.5	56
228	Determination of DNA-base orientation on carbon nanotubes through directional optical absorbance. <i>Nano Letters</i> , <b>2007</b> , 7, 2312-6	11.5	56
227	A molecular picture of hydrophilic and hydrophobic interactions from ab initio density functional theory calculations. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 7617-7620	3.9	55
226	Consistent picture for the wetting structure of water/Ru(0001). <i>Chemical Physics Letters</i> , <b>2005</b> , 402, 384-388	3.8	54
225	Side-group chemical gating via reversible optical and electric control in a single molecule transistor. <i>Nature Communications</i> , <b>2019</b> , 10, 1450	17.4	53
224	Flexible strain sensors with high performance based on metallic glass thin film. <i>Applied Physics Letters</i> , <b>2017</b> , 111, 121906	3.4	50
223	Cooperativity in Surface Bonding and Hydrogen Bonding of Water and Hydroxyl at Metal Surfaces. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 10240-10248	3.8	46
222	Photoinduced Nonequilibrium Topological States in Strained Black Phosphorus. <i>Physical Review Letters</i> , <b>2018</b> , 120, 237403	7.4	45
221	First-principles studies of cation-doped spinel LiMn <sub>2</sub> O <sub>4</sub> for lithium ion batteries. <i>Physical Review B</i> , <b>2003</b> , 67,	3.3	44
220	Water printing of ferroelectric polarization. <i>Nature Communications</i> , <b>2018</b> , 9, 3809	17.4	44
219	Transport behavior of water molecules through two-dimensional nanopores. <i>Journal of Chemical Physics</i> , <b>2014</b> , 141, 18C528	3.9	43
218	Nonlinear Rashba spin splitting in transition metal dichalcogenide monolayers. <i>Nanoscale</i> , <b>2016</b> , 8, 17854-17860	3.7	41
217	Novel Excitonic Solar Cells in Phosphorene-TiO <sub>2</sub> Heterostructures with Extraordinary Charge Separation Efficiency. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 1880-7	6.4	41
216	Controlling Adsorption Structure of Eosin Y Dye on Nanocrystalline TiO <sub>2</sub> Films for Improved Photovoltaic Performances. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 14659-14666	3.8	40
215	Water adsorption on a NaCl (001) surface: A density functional theory study. <i>Physical Review B</i> , <b>2006</b> , 74,	3.3	40
214	Field and temperature dependence of intrinsic diamagnetism in graphene: Theory and experiment. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	39

213	D- $\pi$ A dye system containing cyano-benzoic acid as anchoring group for dye-sensitized solar cells. <i>Langmuir</i> , <b>2011</b> , 27, 14248-52	4	39
212	Intrinsic valley polarization of magnetic VSe monolayers. <i>Journal of Physics Condensed Matter</i> , <b>2017</b> , 29, 255501	1.8	37
211	New Pathway for Hot Electron Relaxation in Two-Dimensional Heterostructures. <i>Nano Letters</i> , <b>2018</b> , 18, 6057-6063	11.5	37
210	Mechanisms for ultrafast nonradiative relaxation in electronically excited eumelanin constituents. <i>Biophysical Journal</i> , <b>2008</b> , 95, 4396-402	2.9	37
209	Selective adsorption and electronic interaction of F16CuPc on epitaxial graphene. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	36
208	Screening Magnetic Two-Dimensional Atomic Crystals with Nontrivial Electronic Topology. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 6709-6715	6.4	35
207	Photoexcitation in Solids: First-Principles Quantum Simulations by Real-Time TDDFT. <i>Advanced Theory and Simulations</i> , <b>2018</b> , 1, 1800055	3.5	34
206	Modeling charge recombination in dye-sensitized solar cells using first-principles electron dynamics: effects of structural modification. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 17187-94	3.6	34
205	Tuning solid surfaces from hydrophobic to superhydrophilic by submonolayer surface modification. <i>Physical Review Letters</i> , <b>2006</b> , 97, 036107	7.4	33
204	Transparent proton transport through a two-dimensional nanomesh material. <i>Nature Communications</i> , <b>2019</b> , 10, 3971	17.4	32
203	Dynamical properties and the proton transfer mechanism in the wetting water layer on Pt(111). <i>Surface Science</i> , <b>2005</b> , 575, 300-306	1.8	32
202	Benign Interfacial Iodine Vacancies in Perovskite Solar Cells. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 5905-5913	3.8	30
201	Controlling states of water droplets on nanostructured surfaces by design. <i>Nanoscale</i> , <b>2017</b> , 9, 18240-18245	7.5	30
200	Anomalous magnetism in strained La(1-x)Sr(x)CoO <sub>3</sub> epitaxial films (0 $\leq$ x $\leq$ 0.5). <i>Scientific Reports</i> , <b>2014</b> , 4, 6206	4.9	30
199	Laser picoscopy of valence electrons in solids. <i>Nature</i> , <b>2020</b> , 583, 55-59	50.4	30
198	Strain-induced defect superstructure on the SrTiO <sub>3</sub> (110) surface. <i>Physical Review Letters</i> , <b>2013</b> , 111, 056101	7.4	30
197	Regulating energy transfer of excited carriers and the case for excitation-induced hydrogen dissociation on hydrogenated graphene. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2013</b> , 110, 908-11	11.5	29
196	Theoretical investigation of the C <sub>60</sub> /copper phthalocyanine organic photovoltaic heterojunction. <i>Nano Research</i> , <b>2012</b> , 5, 248-257	10	29

195	Three-dimensional metal-intercalated covalent organic frameworks for near-ambient energy storage. <i>Scientific Reports</i> , <b>2013</b> , 3, 1882	4.9	28
194	Precise identification and manipulation of adsorption geometry of donor-acceptor dye on nanocrystalline TiO <sub>2</sub> films for improved photovoltaics. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2014</b> , 6, 22359-69	9.5	28
193	Turning on and off the rotational oscillation of a single porphine molecule by molecular charge state. <i>ACS Nano</i> , <b>2012</b> , 6, 4132-6	16.7	28
192	Reversible transition between thermodynamically stable phases with low density of oxygen vacancies on the SrTiO <sub>3</sub> (110) surface. <i>Physical Review Letters</i> , <b>2011</b> , 107, 036103	7.4	28
191	Quantum plasmonics: Symmetry-dependent plasmon-molecule coupling and quantized photoconductances. <i>Physical Review B</i> , <b>2012</b> , 86,	3.3	28
190	Structural, electronic, and optical properties of representative Cu-flavonoid complexes. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 6478-83	3.4	27
189	Dissolution dynamics of NaCl nanocrystal in liquid water. <i>Physical Review E</i> , <b>2005</b> , 72, 012602	2.4	27
188	Multilayered silicene: the bottom-up approach for a weakly relaxed Si(111) with Dirac surface states. <i>Nanoscale</i> , <b>2015</b> , 7, 15880-5	7.7	26
187	Formation and interaction of hydrated alkali metal ions at the graphite-water interface. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 014708	3.9	26
186	Ultrafast charge ordering by self-amplified exciton-phonon dynamics in TiSe. <i>Nature Communications</i> , <b>2020</b> , 11, 43	17.4	26
185	Ab initio evidence for nonthermal characteristics in ultrafast laser melting. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	26
184	Structure and quantum well states in silicene nanoribbons on Ag(110). <i>Surface Science</i> , <b>2016</b> , 645, 74-79	1.8	25
183	Effective Hamiltonian for FeAs-based superconductors. <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	25
182	Chen et al. reply. <i>Physical Review Letters</i> , <b>2013</b> , 110, 229702	7.4	24
181	Photocontrol of charge injection/extraction at electrode/semiconductor interfaces for high-photoresponsivity organic transistors. <i>Journal of Materials Chemistry C</i> , <b>2016</b> , 4, 5289-5296	7.1	24
180	Coexistence of Different Charge-Transfer Mechanisms in the Hot-Carrier Dynamics of Hybrid Plasmonic Nanomaterials. <i>Nano Letters</i> , <b>2019</b> , 19, 3187-3193	11.5	23
179	Atomistic nature of NaCl nucleation at the solid-liquid interface. <i>Journal of Chemical Physics</i> , <b>2007</b> , 126, 044708	3.9	23
178	Integrated Plasmonics: Broadband Dirac Plasmons in Borophene. <i>Physical Review Letters</i> , <b>2020</b> , 125, 116802	7.4	23

177	Plasmon-Induced Ultrafast Hydrogen Production in Liquid Water. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 63-69	6.4	23
176	Ideal type-II Weyl phonons in wurtzite CuI. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	22
175	Plasmon-induced dynamics of H <sub>2</sub> splitting on a silver atomic chain. <i>Applied Physics Letters</i> , <b>2015</b> , 107, 083102	3.4	22
174	Basic science of water: Challenges and current status towards a molecular picture. <i>Nano Research</i> , <b>2015</b> , 8, 3085-3110	10	21
173	The effect of moiré superstructures on topological edge states in twisted bismuthene homojunctions. <i>Science Advances</i> , <b>2020</b> , 6, eaba2773	14.3	21
172	Two-dimensional hydration shells of alkali metal ions at a hydrophobic surface. <i>Journal of Chemical Physics</i> , <b>2004</b> , 121, 12572-6	3.9	21
171	Ultrafast Broadband Charge Collection from Clean Graphene/CHNHPbI Interface. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 14952-14957	16.4	21
170	Quinoid conjugated dye designed for efficient sensitizer in dye sensitized solar cells. <i>Chemical Physics Letters</i> , <b>2013</b> , 586, 97-99	2.5	20
169	Plasmon-driven sub-picosecond breathing of metal nanoparticles. <i>Nanoscale</i> , <b>2017</b> , 9, 12391-12397	7.7	20
168	Exotic thermoelectric behavior in nitrogenated holey graphene. <i>RSC Advances</i> , <b>2017</b> , 7, 25803-25810	3.7	19
167	Meng et al. Reply:. <i>Physical Review Letters</i> , <b>2003</b> , 91,	7.4	19
166	Spin-Orientation-Dependent Topological States in Two-Dimensional Antiferromagnetic NiTiS Monolayers. <i>Nano Letters</i> , <b>2019</b> , 19, 3321-3326	11.5	18
165	Universal Scaling of Intrinsic Resistivity in Two-Dimensional Metallic Borophene. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 4585-4589	16.4	18
164	Wetting behavior of water on silicon carbide polar surfaces. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 28033-28039	3.6	18
163	Superconductivity in dense carbon-based materials. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	18
162	Cooperative evolution of intraband and interband excitations for high-harmonic generation in strained MoS <sub>2</sub> . <i>Physical Review B</i> , <b>2019</b> , 99,	3.3	17
161	Flat AgTe Honeycomb Monolayer on Ag(111). <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 1866-1871	6.4	17
160	Intrinsic electronic transport and thermoelectric power factor in n-type doped monolayer MoS <sub>2</sub> . <i>New Journal of Physics</i> , <b>2018</b> , 20, 043009	2.9	17



159	Magnetic Dirac fermions and Chern insulator supported on pristine silicon surface. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	17
158	Water wettability of close-packed metal surfaces. <i>Journal of Chemical Physics</i> , <b>2007</b> , 127, 244710	3.9	17
157	Electronic Structures and Catalytic Activities of Niobium Oxides as Electrocatalysts in Liquid-Junction Photovoltaic Devices. <i>Solar Rrl</i> , <b>2020</b> , 4, 1900430	7.1	17
156	Multigap anisotropic superconductivity in borophenes. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	17
155	Recent progresses in real-time local-basis implementation of time dependent density functional theory for electron-nucleus dynamics. <i>Computational Materials Science</i> , <b>2016</b> , 112, 478-486	3.2	16
154	Effects of line defects on the electronic and optical properties of strain-engineered WO <sub>3</sub> thin films. <i>Journal of Materials Chemistry C</i> , <b>2017</b> , 5, 11694-11699	7.1	16
153	Probing Nonequilibrium Dynamics of Photoexcited Polarons on a Metal-Oxide Surface with Atomic Precision. <i>Physical Review Letters</i> , <b>2020</b> , 124, 206801	7.4	16
152	Hidden spin polarization in the 1 T -phase layered transition-metal dichalcogenides MX <sub>2</sub> (M = Zr, Hf; X = S, Se, Te). <i>Science Bulletin</i> , <b>2018</b> , 63, 85-91	10.6	16
151	Photoexcitation Induced Quantum Dynamics of Charge Density Wave and Emergence of a Collective Mode in 1-TaS. <i>Nano Letters</i> , <b>2019</b> , 19, 6027-6034	11.5	16
150	Water wetting on representative metal surfaces: Improved description from van der Waals density functionals. <i>Chemical Physics Letters</i> , <b>2012</b> , 521, 161-166	2.5	16
149	Prediction of two-dimensional electron gas mediated magnetoelectric coupling at ferroelectric PbTiO <sub>3</sub> /SrTiO <sub>3</sub> heterostructures. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	16
148	Dirac cone pairs in silicene induced by interface Si-Ag hybridization: A first-principles effective band study. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	16
147	Phonon thermal transport in a class of graphene allotropes from first principles. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 15980-15985	3.6	16
146	High thermopower and potential thermoelectric properties of crystalline LiH and NaH. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	15
145	An Iron-Porphyrin Complex with Large Easy-Axis Magnetic Anisotropy on Metal Substrate. <i>ACS Nano</i> , <b>2017</b> , 11, 11402-11408	16.7	15
144	Long-Lived Multifunctional Superhydrophobic Heterostructure Via Molecular Self-Supply. <i>Advanced Materials Interfaces</i> , <b>2016</b> , 3, 1500727	4.6	15
143	Bis(pyrazol-1-yl)methane as Non-Chromophoric Ancillary Ligand for Charged Bis-Cyclometalated Iridium(III) Complexes. <i>European Journal of Inorganic Chemistry</i> , <b>2012</b> , 2012, 3209-3215	2.3	15
142	Water transport through subnanopores in the ultimate size limit: Mechanism from molecular dynamics. <i>Nano Research</i> , <b>2019</b> , 12, 587-592	10	15

141	Identifying Few-Molecule Water Clusters with High Precision on Au(111) Surface. <i>ACS Nano</i> , <b>2018</b> , 12, 6452-6457	16.7	15
140	Superstructure-Induced Splitting of Dirac Cones in Silicene. <i>Physical Review Letters</i> , <b>2019</b> , 122, 196801	7.4	14
139	A molecular dynamics study of hydration and dissolution of NaCl nanocrystal in liquid water. <i>Journal of Physics Condensed Matter</i> , <b>2006</b> , 18, 10165-10177	1.8	14
138	Ultrafast Optical Modulation of Harmonic Generation in Two-Dimensional Materials. <i>Nano Letters</i> , <b>2020</b> , 20, 8053-8058	11.5	14
137	Carbene-mediated self-assembly of diamondoids on metal surfaces. <i>Nanoscale</i> , <b>2016</b> , 8, 8966-75	7.7	14
136	Vibrational relaxation dynamics of the nitrogen-vacancy center in diamond. <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	13
135	Ultrasmall silver nanopores fabricated by femtosecond laser pulses. <i>Nano Letters</i> , <b>2011</b> , 11, 3251-7	11.5	13
134	Tunable electron-phonon coupling superconductivity in platinum diselenide. <i>Physical Review Materials</i> , <b>2017</b> , 1,	3.2	13
133	Giant enhancement of optical nonlinearity in two-dimensional materials by multiphoton-excitation resonance energy transfer from quantum dots. <i>Nature Photonics</i> ,	33.9	13
132	High-Efficiency Selective Electron Tunnelling in a Heterostructure Photovoltaic Diode. <i>Nano Letters</i> , <b>2016</b> , 16, 3600-6	11.5	13
131	Momentum-resolved TDDFT algorithm in atomic basis for real time tracking of electronic excitation. <i>Journal of Chemical Physics</i> , <b>2018</b> , 149, 154104	3.9	13
130	Optical properties of clusters and molecules from real-time time-dependent density functional theory using a self-consistent field. <i>Molecular Physics</i> , <b>2010</b> , 108, 1829-1844	1.7	12
129	Improving Photovoltaic Stability and Performance of Perovskite Solar Cells by Molecular Interface Engineering. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 1219-1225	3.8	12
128	Hexagonal Monolayer Ice without Shared Edges. <i>Physical Review Letters</i> , <b>2018</b> , 121, 256001	7.4	12
127	Water nanostructure formation on oxide probed in situ by optical resonances. <i>Science Advances</i> , <b>2019</b> , 5, eaax6973	14.3	11
126	"H <sub>2</sub> sponge": pressure as a means for reversible high-capacity hydrogen storage in nanoporous Ca-intercalated covalent organic frameworks. <i>Nanoscale</i> , <b>2015</b> , 7, 6319-24	7.7	11
125	Tunable hydrophobicity on fractal and micro-nanoscale hierarchical fracture surface of metallic glasses. <i>Materials and Design</i> , <b>2016</b> , 95, 612-617	8.1	11
124	Suppression of nonradiative recombination in ionic insulators by defects: Role of fast electron trapping in Tl-doped CsI. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	11

123	Initial interactions between water molecules and Ti-adsorbed carbon nanotubes. <i>Applied Physics Letters</i> , <b>2007</b> , 91, 161906	3.4	11
122	Low lattice thermal conductivity and excellent thermoelectric behavior in LiSb and LiBi. <i>Journal of Physics Condensed Matter</i> , <b>2018</b> , 30, 425401	1.8	11
121	Tuning magnetic splitting of zigzag graphene nanoribbons by edge functionalization with hydroxyl groups. <i>Journal of Applied Physics</i> , <b>2015</b> , 117, 113902	2.5	10
120	Two-dimensional silicon-carbon hybrids with a honeycomb lattice: New family for two-dimensional photovoltaic materials. <i>Science China: Physics, Mechanics and Astronomy</i> , <b>2015</b> , 58, 1	3.6	10
119	Silicene: from monolayer to multilayer [A concise review. <i>Chinese Physics B</i> , <b>2015</b> , 24, 086102	1.2	10
118	Toward attosecond control of electron dynamics in two-dimensional materials. <i>Applied Physics Letters</i> , <b>2020</b> , 116, 043101	3.4	10
117	Plasmon-induced nonlinear response of silver atomic chains. <i>Nanoscale</i> , <b>2018</b> , 10, 8600-8605	7.7	10
116	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> , <b>2019</b> , 116, 23410-23415	11.5	10
115	Dye Sensitized Solar Cells Principles and New Design <b>2011</b> ,		10
114	Low lattice thermal conductivity and good thermoelectric performance of cinnabar. <i>Physical Review Materials</i> , <b>2017</b> , 1,	3.2	10
113	Two-gap and three-gap superconductivity in AlB <sub>2</sub> -based films. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	9
112	Hard BN Clathrate Superconductors. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 2554-2560	6.4	9
111	Atomistic mechanism of charge separation upon photoexcitation at the dye-semiconductor interface for photovoltaic applications. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 13196-201	3.6	9
110	First-principles dynamics of photoexcited molecules and materials towards a quantum description. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2021</b> , 11, e1492	7.9	9
109	Pressure induced excellent thermoelectric behavior in skutterudites CoSb and IrSb. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 851-858	3.6	8
108	Reducing Anomalous Hysteresis in Perovskite Solar Cells by Suppressing the Interfacial Ferroelectric Order. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2020</b> , 12, 12275-12284	9.5	8
107	Optical Properties of Single- and Double-Functionalized Small Diamondoids. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 3583-3593	2.8	8
106	Inducing Transient Charge State of a Single Water Cluster on Cu(111) Surface. <i>ACS Nano</i> , <b>2016</b> , 10, 4489-4507	16.7	8

105	Transparency in graphene mediated evaporation. <i>2D Materials</i> , <b>2018</b> , 5, 041001	5.9	8
104	Ice II-like Monolayer Ice Grown on Graphite Surface. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 20297-20303	3.3	8
103	Extreme nonlinear strong-field photoemission from carbon nanotubes. <i>Nature Communications</i> , <b>2019</b> , 10, 4891	17.4	8
102	Superconducting transition of FeSe/SrTiO <sub>3</sub> induced by adsorption of semiconducting organic molecules. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	8
101	Quantum simulation of molecular interaction and dynamics at surfaces. <i>Frontiers of Physics</i> , <b>2011</b> , 6, 294-308	3.7	8
100	Fermionic Analogue of High Temperature Hawking Radiation in Black Phosphorus. <i>Chinese Physics Letters</i> , <b>2020</b> , 37, 067101	1.8	8
99	Manipulating Weyl quasiparticles by orbital-selective photoexcitation in WTe. <i>Nature Communications</i> , <b>2021</b> , 12, 1885	17.4	8
98	Nonadiabatic Dynamics of Photocatalytic Water Splitting on A Polymeric Semiconductor. <i>Nano Letters</i> , <b>2021</b> , 21, 6449-6455	11.5	8
97	The 2021 ultrafast spectroscopic probes of condensed matter roadmap. <i>Journal of Physics Condensed Matter</i> , <b>2021</b> , 33,	1.8	8
96	Free-Standing Single-Molecule Thick Crystals Consisting of Linear Long-Chain Polymers. <i>Nano Letters</i> , <b>2017</b> , 17, 1655-1659	11.5	7
95	A modified Wenzel model for water wetting on van der Waals layered materials with topographic surfaces. <i>Nanoscale</i> , <b>2017</b> , 9, 3843-3849	7.7	7
94	Visualizing molecular orientational ordering and electronic structure in C <sub>60</sub> fulleride films. <i>Physical Review B</i> , <b>2020</b> , 101,	3.3	7
93	Phonon thermal transport in monolayer FeB <sub>2</sub> from first principles. <i>Computational Materials Science</i> , <b>2018</b> , 147, 132-136	3.2	7
92	Spin-polarized valley Hall effect in ultrathin silicon nanomembrane via interlayer antiferromagnetic coupling. <i>2D Materials</i> , <b>2016</b> , 3, 035026	5.9	7
91	Promote water photosplitting via tuning quantum well states in supported metal clusters. <i>Physical Review B</i> , <b>2012</b> , 86,	3.3	7
90	Effect of symmetry breaking on the optical absorption of semiconductor nanoparticles. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	7
89	Is the nature of magnetic order in copper-oxides and in iron-pnictides different?. <i>Solid State Communications</i> , <b>2010</b> , 150, 62-65	1.6	7
88	Image force effects on trapezoidal barrier parameters in metal-insulator-metal tunnel junctions. <i>Thin Solid Films</i> , <b>2003</b> , 436, 292-297	2.2	7

87	Controlling catalytic activity of gold cluster on MgO thin film for water splitting. <i>Physical Review Materials</i> , <b>2017</b> , 1,	3.2	7
86	Indirect to Direct Charge Transfer Transition in Plasmon-Enabled CO Photoreduction. <i>Advanced Science</i> , <b>2021</b> , 9, e2102978	13.6	7
85	Engineering Dirac states in graphene: Coexisting type-I and type-II Floquet-Dirac fermions. <i>Physical Review B</i> , <b>2019</b> , 99,	3.3	6
84	Quartic anharmonicity and anomalous thermal conductivity in cubic antiperovskites A <sub>3</sub> BO (A=K, Rb; B=Br, Au). <i>Physical Review B</i> , <b>2020</b> , 101,	3.3	6
83	A combined experimental and theoretical investigation of donor and acceptor interface in efficient aqueous-processed polymer/nanocrystal hybrid solar cells. <i>Science China Chemistry</i> , <b>2018</b> , 61, 437-443	7.9	6
82	The excellent TE performance of photoelectric material CdSe along with a study of Zn(Cd)Se and Zn(Cd)Te based on first-principles.. <i>RSC Advances</i> , <b>2019</b> , 9, 25471-25479	3.7	6
81	Sequential assembly of metal-free phthalocyanine on few-layer epitaxial graphene mediated by thickness-dependent surface potential. <i>Nano Research</i> , <b>2012</b> , 5, 543-549	10	6
80	Atomically Precise Engineering of Single-Molecule Stereoelectronic Effect. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 12274-12278	16.4	6
79	Tunable magnetic moment and potential half-metal behavior of Fe-nanostructure-embedded graphene perforation. <i>Carbon</i> , <b>2016</b> , 107, 268-272	10.4	5
78	Scanning tunneling microscopy investigations of unoccupied surface states in two-dimensional semiconducting Bi <sub>2</sub> Se <sub>3</sub> /Bi/Si(111) surface. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 20188-20193	3.6	5
77	Direct imaging of surface states hidden in the third layer of Si (111)-7 $\times$ 7 surface by pz-wave tip. <i>Applied Physics Letters</i> , <b>2018</b> , 113, 031604	3.4	5
76	High-Efficiency Photovoltaic Conversion at Selective Electron Tunneling Heterointerfaces. <i>Advanced Electronic Materials</i> , <b>2017</b> , 3, 1700211	6.4	5
75	Phase Transition Photodetection in Charge Density Wave Tantalum Disulfide. <i>Nano Letters</i> , <b>2020</b> , 20, 6725-6731	11.5	5
74	Low thermal conductivity and good thermoelectric performance in mercury chalcogenides. <i>Computational Materials Science</i> , <b>2020</b> , 185, 109960	3.2	5
73	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
72	Dual-gated single-molecule field-effect transistors beyond Moore's law.. <i>Nature Communications</i> , <b>2022</b> , 13, 1410	17.4	5
71	Fe on Sb(111): Potential Two-Dimensional Ferromagnetic Superstructures. <i>ACS Nano</i> , <b>2017</b> , 11, 2143-2146	16.7	4
70	Orbital dependent interaction of quantum well states for catalytic water splitting. <i>New Journal of Physics</i> , <b>2015</b> , 17, 013023	2.9	4

69	Universal Scaling of Intrinsic Resistivity in Two-Dimensional Metallic Borophene. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 4675-4679	3.6	4
68	New sensitizers containing amide moieties as electron-accepting and anchoring groups for dye-sensitized solar cells. <i>RSC Advances</i> , <b>2016</b> , 6, 74039-74045	3.7	4
67	Band evolution of two-dimensional transition metal dichalcogenides under electric fields. <i>Applied Physics Letters</i> , <b>2019</b> , 115, 083104	3.4	4
66	Kondo effect mediated topological protection: Co on Sb(111). <i>ACS Nano</i> , <b>2014</b> , 8, 11576-82	16.7	4
65	Dye-sensitized solar cells: Atomic scale investigation of interface structure and dynamics. <i>Chinese Physics B</i> , <b>2014</b> , 23, 086801	1.2	4
64	Interaction of DNA with CNTs: Properties and Prospects for Electronic Sequencing	67-96	4
63	Exactly solvable model for metal-insulator-metal stepped boundary tunnel junctions. <i>Thin Solid Films</i> , <b>2002</b> , 414, 136-142	2.2	4
62	Single-water-dipole-layer-driven Reversible Charge Order Transition in 1-TaS. <i>Nano Letters</i> , <b>2020</b> , 20, 8854-8860	11.5	4
61	Electric Field Tunable Ultrafast Interlayer Charge Transfer in Graphene/WS Heterostructure. <i>Nano Letters</i> , <b>2021</b> , 21, 4403-4409	11.5	4
60	Mechanism and modulation of terahertz generation from a semimetal-graphite. <i>Scientific Reports</i> , <b>2016</b> , 6, 22798	4.9	4
59	Quantum dynamics simulations: combining path integral nuclear dynamics and real-time TDDFT. <i>Electronic Structure</i> , <b>2019</b> , 1, 044005	2.6	4
58	Infrared spectroscopic study on lattice dynamics in CaFeO <sub>3</sub> . <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	3
57	Self-assembly of glycine on Cu(001): the effect of temperature and polarity. <i>RSC Advances</i> , <b>2017</b> , 7, 4116-4123	3.7	3
56	Real-Space Imaging of Orbital Selectivity on SrTiO(001) Surface. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 37279-37284	9.5	3
55	Comprehensive calculations and prominent thermoelectric properties of Li <sub>3</sub> P and Li <sub>3</sub> As. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2019</b> , 383, 2802-2808	2.3	3
54	Reply to Comment on Ab initio evidence for nonthermal characteristics in ultrafast laser melting. <i>Physical Review B</i> , <b>2019</b> , 99,	3.3	3
53	Distribution and concentration of surface oxygen vacancy of TiO <sub>2</sub> and its photocatalytic activity. <i>Journal Physics D: Applied Physics</i> , <b>2020</b> , 53, 424001	3	3
52	Emergence of d-orbital magnetic Dirac fermions in a MoS <sub>2</sub> monolayer with squared pentagon structure. <i>Physical Review B</i> , <b>2020</b> , 101,	3.3	3

51	Surface confined quantum well state in MoS <sub>2</sub> (0001) thin film. <i>Applied Physics Letters</i> , <b>2015</b> , 107, 161602	3.4	3
50	Observation of One-Dimensional Dirac Fermions in Silicon Nanoribbons.. <i>Nano Letters</i> , <b>2022</b> , 22, 695-701	11.5	3
49	Screening single-atom catalysts for methane activation: Al <sub>2</sub> O <sub>3</sub> (0001)-supported Ni. <i>Physical Review Materials</i> , <b>2017</b> , 1,	3.2	3
48	Plasmon-Mediated CO <sub>2</sub> Photoreduction via Indirect Charge Transfer on Small Silver Nanoclusters. <i>Journal of Physical Chemistry C</i> ,	3.8	3
47	The structural, electronic and optic properties in a series of M <sub>2</sub> XY (M = Ga, In; X,Y = S, Se, Te) Janus monolayer materials based on GW and the Bethe-Salpeter equation. <i>European Physical Journal B</i> , <b>2020</b> , 93, 1	1.2	3
46	Manipulation of the Magnetic Anisotropy of Single Mn Atom via Molecular Ligands. <i>Nano Letters</i> , <b>2021</b> , 21, 3566-3572	11.5	3
45	Theoretical Insights into Ultrafast Dynamics in Quantum Materials. <i>Ultrafast Science</i> , <b>2022</b> , 2022, 1-16		3
44	Effect of single point defect on local properties in BiFeO <sub>3</sub> thin film. <i>Acta Materialia</i> , <b>2019</b> , 170, 132-137	8.4	2
43	MgB <sub>4</sub> trilayer film: A four-gap superconductor. <i>Physical Review B</i> , <b>2020</b> , 101,	3.3	2
42	Rotational and Vibrational Excitations of a Single Water Molecule by Inelastic Electron Tunneling Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 1650-1655	6.4	2
41	Giant photoinduced lattice distortion in oxygen vacancy ordered SrCoO <sub>2.5</sub> thin films. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	2
40	Theoretical Models of Eumelanin Protomolecule and Its Photoprotection Mechanism. <i>Biophysical Journal</i> , <b>2009</b> , 96, 300a	2.9	2
39	The pressure induced phase transition of confined water from ab initio molecular dynamics simulation. <i>Journal of Physics Condensed Matter</i> , <b>2004</b> , 16, 8851-8859	1.8	2
38	Optical Control of Multistage Phase Transition via Phonon Coupling in MoTe <sub>2</sub> .. <i>Physical Review Letters</i> , <b>2022</b> , 128, 015702	7.4	2
37	Plasmon-mediated photodecomposition of NH <sub>3</sub> via intramolecular charge transfer. <i>Nano Research</i> ,	10	2
36	Viable substrates for the honeycomb-borophene growth. <i>Physical Review Materials</i> , <b>2021</b> , 5,	3.2	2
35	The valley degree of freedom of an electron. <i>Wuli Xuebao/Acta Physica Sinica</i> , <b>2015</b> , 64, 187301	0.6	2
34	Anomalous electronic and thermoelectric transport properties in cubic Rb <sub>3</sub> AuO antiperovskite. <i>Physical Review B</i> , <b>2020</b> , 102,	3.3	2

33	A comprehensive phonon thermal transport study of 2D hexagonal MX <sub>2</sub> and orthorhombic M <sub>2</sub> X <sub>3</sub> (M = Ni, Pd; X = S, Se and Te). <i>Materials Today Communications</i> , <b>2020</b> , 25, 101441	2.5	2
32	Role of Explicitly Included Solvents on Ultrafast Electron Injection and Recombination Dynamics at TiO <sub>2</sub> /Dye Interfaces. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2020</b> , 12, 49174-49181	9.5	2
31	Thermally induced band hybridization in bilayer-bilayer MoS <sub>2</sub> /WS <sub>2</sub> heterostructure*. <i>Chinese Physics B</i> , <b>2021</b> , 30, 057801	1.2	2
30	Dynamic defect as nonradiative recombination center in semiconductors. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	2
29	Quartic anharmonicity and ultra-low lattice thermal conductivity of alkali antimonide compounds M <sub>3</sub> Sb (M = K, Rb and Cs). <i>International Journal of Energy Research</i> , <b>2021</b> , 45, 6958-6965	4.5	2
28	Tuning of the oxygen vacancies in LaCoO <sub>3</sub> films at the atomic scale. <i>Applied Physics Letters</i> , <b>2021</b> , 118, 081602	3.4	2
27	Direct observation of atomic-level fractal structure in a metallic glass membrane. <i>Science Bulletin</i> , <b>2021</b> ,	10.6	2
26	Probing Laser-Induced Plasma Generation in Liquid Water. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 10382-10388	16.4	2
25	Inspecting the nonbonding and antibonding orbitals in a surface-supported metal-organic framework. <i>Chemical Communications</i> , <b>2021</b> , 57, 4580-4583	5.8	2
24	All-Silicon Switchable Magnetoelectric Effect through Interlayer Exchange Coupling. <i>ChemPhysChem</i> , <b>2017</b> , 18, 1916-1920	3.2	1
23	Ab initio study on anisotropic thermoelectric transport in ternary pnictide KZnP. <i>JPhys Materials</i> , <b>2019</b> , 2, 024001	4.2	1
22	Robust quantum spin Hall state and quantum anomalous Hall state in graphenelike BC <sub>3</sub> with adatoms. <i>New Journal of Physics</i> , <b>2018</b> , 20, 073047	2.9	1
21	Macroscopic superhydrophobicity achieved by atomic decoration with silicones. <i>Journal of Chemical Physics</i> , <b>2018</b> , 149, 014706	3.9	1
20	The High-Temperature Oxidation of Nb-40Ti-15Al and the Effect of Cr Alloying and Silicide Diffusion Coatings. <i>Materials Research Society Symposia Proceedings</i> , <b>1994</b> , 364, 1327		1
19	Tracking photocarrier-enhanced electron-phonon coupling in nonequilibrium. <i>Npj Quantum Materials</i> , <b>2022</b> , 7,	5	1
18	Epitaxial growth and band structure of antiferromagnetic Mott insulator CeOI. <i>Physical Review Materials</i> , <b>2020</b> , 4,	3.2	1
17	Molecular transport across a two-dimensional nanomesh membrane-graphdiyne. <i>Journal Physics D: Applied Physics</i> , <b>2020</b> , 53, 493003	3	1
16	Plasmon-Induced Water Splitting on Ag-Alloyed Pt Single-Atom Catalysts. <i>Frontiers in Chemistry</i> , <b>2021</b> , 9, 742794	5	1



15	First-principles study of phonon thermal transport in III-V group graphenelike materials. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , <b>2020</b> , 38, 062202	2.9	1
14	Ultra-low lattice thermal conductivity and high thermoelectric efficiency of K <sub>3</sub> AuO. <i>Journal of Applied Physics</i> , <b>2021</b> , 130, 045101	2.5	1
13	Monolayer puckered pentagonal VTe <sub>2</sub> : An emergent two-dimensional ferromagnetic semiconductor with multiferroic coupling. <i>Nano Research</i> , 1	10	1
12	Calibrating Out-of-Equilibrium Electron-Phonon Couplings in Photoexcited MoS <sub>2</sub> . <i>Nano Letters</i> ,	11.5	1
11	Water on surfaces from first-principles molecular dynamics. <i>Chinese Physics B</i> , <b>2020</b> , 29, 116804	1.2	0
10	Creation of a novel inverted charge density wave state.. <i>Structural Dynamics</i> , <b>2022</b> , 9, 014501	3.2	0
9	Unravelling a Zigzag Pathway for Hot Carrier Collection with Graphene Electrode. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 2886-2891	6.4	0
8	High-Throughput Screening of Element-Doped Carbon Nanotubes Toward an Optimal One-Dimensional Superconductor. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 6667-6675	6.4	0
7	Water overlayers on Cu(110) studied by van der Waals density functionals <b>2012</b> , 67-75		
6	Calibrating the unphysical divergence in TDDFT+U simulations of a correlated oxide. <i>Computational Materials Science</i> , <b>2022</b> , 203, 111167	3.2	
5	Nanosession: 2D Electron Systems - Correlation Effects and Transport 81-88		
4	Atomically Precise Engineering of Single-Molecule Stereoelectronic Effect. <i>Angewandte Chemie</i> , <b>2021</b> , 133, 12382-12386	3.6	
3	Low thermal conductivity and good thermoelectric performance in mercury chalcogenides. <i>Computational Materials Science</i> , <b>2021</b> , 188, 110192	3.2	
2	Local Kondo scattering in 4d-electron RuO nanoclusters on atomically-resolved ultrathin SrRuO films. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 22526-22531	3.6	
1	Non-Hermitian topological states in 2D line-graph lattices: evolving triple exceptional points on reciprocal line graphs. <i>New Journal of Physics</i> , <b>2021</b> , 23, 123038	2.9	