

## List of Publications by Citations

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

91 papers	5,445 citations	41 h-index	73 g-index
96 ext. papers	6,377 ext. citations	7.5 avg, IF	6.01 L-index

#	Paper	IF	Citations
91	Electronic structure and carrier mobility in graphdiyne sheet and nanoribbons: theoretical predictions. <i>ACS Nano</i> , <b>2011</b> , 5, 2593-600	16.7	697
90	Tunable band gap photoluminescence from atomically thin transition-metal dichalcogenide alloys. <i>ACS Nano</i> , <b>2013</b> , 7, 4610-6	16.7	442
89	First-principles prediction of charge mobility in carbon and organic nanomaterials. <i>Nanoscale</i> , <b>2012</b> , 4, 4348-69	7.7	412
88	Carrier Mobility in Graphyne Should Be Even Larger than That in Graphene: A Theoretical Prediction. <i>Journal of Physical Chemistry Letters</i> , <b>2013</b> , 4, 1443-8	6.4	254
87	Theoretical predictions of size-dependent carrier mobility and polarity in graphene. <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 17728-9	16.4	247
86	Aggregation induced blue-shifted emission--the molecular picture from a QM/MM study. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 5545-52	3.6	138
85	Unravelling Doping Effects on PEDOT at the Molecular Level: From Geometry to Thermoelectric Transport Properties. <i>Journal of the American Chemical Society</i> , <b>2015</b> , 137, 12929-38	16.4	129
84	Supramolecular organic nanofibers with highly efficient and stable visible light photooxidation performance. <i>Applied Catalysis B: Environmental</i> , <b>2017</b> , 202, 289-297	21.8	124
83	MOlecular MAterials Property Prediction Package (MOMAP) 1.0: a software package for predicting the luminescent properties and mobility of organic functional materials. <i>Molecular Physics</i> , <b>2018</b> , 116, 1078-1090	1.7	110
82	CsPbI <sub>2</sub> Cl, All-Inorganic Two-Dimensional Ruddlesden-Popper Mixed Halide Perovskite with Optoelectronic Response. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 11085-11090	16.4	110
81	Intrinsic and Extrinsic Charge Transport in CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> Perovskites Predicted from First-Principles. <i>Scientific Reports</i> , <b>2016</b> , 7, 19968	4.9	103
80	Controlled orientation of perovskite films through mixed cations toward high performance perovskite solar cells. <i>Nano Energy</i> , <b>2016</b> , 27, 87-94	17.1	102
79	Aggregation effects on the optical emission of 1,1,2,3,4,5-hexaphenylsilole (HPS): a QM/MM study. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 9094-104	2.8	92
78	Theoretical Study of Conversion and Decay Processes of Excited Triplet and Singlet States in a Thermally Activated Delayed Fluorescence Molecule. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 13448-13456	3.8	91
77	Tunable Electronic Properties of Two-Dimensional Transition Metal Dichalcogenide Alloys: A First-Principles Prediction. <i>Journal of Physical Chemistry Letters</i> , <b>2014</b> , 5, 285-91	6.4	77
76	Formation of naphthalene, indene, and benzene from cyclopentadiene pyrolysis: a DFT study. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 4719-25	2.8	76
75	Modeling thermoelectric transport in organic materials. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 16505-20	3.6	75

74	Visible-light-switched electron transfer over single porphyrin-metal atom center for highly selective electroreduction of carbon dioxide. <i>Nature Communications</i> , <b>2019</b> , 10, 3844	17.4	66
73	Search for Organic Thermoelectric Materials with High Mobility: The Case of 2,7-Dialkyl[1]benzothieno[3,2-b][1]benzothiophene Derivatives. <i>Chemistry of Materials</i> , <b>2014</b> , 26, 2669-2677	2.6	66
72	Indirect-to-Direct Band Gap Crossover in Few-Layer Transition Metal Dichalcogenides: A Theoretical Prediction. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 21866-21870	3.8	66
71	Influence of alkyl side-chain length on the carrier mobility in organic semiconductors: herringbone vs. $\pi\pi$ stacking. <i>Journal of Materials Chemistry C</i> , <b>2016</b> , 4, 4546-4555	7.1	64
70	Water transport and purification in nanochannels controlled by asymmetric wettability. <i>Small</i> , <b>2011</b> , 7, 2225-31	11	61
69	Supramolecular catalyst functions in catalytic amount: cucurbit[8]uril accelerates the photodimerization of Brooker's merocyanine. <i>Chemical Science</i> , <b>2017</b> , 8, 8357-8361	9.4	60
68	Spectroscopic Signature of the Aggregation-Induced Emission Phenomena Caused by Restricted Nonradiative Decay: A Theoretical Proposal. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 5040-5047	3.8	59
67	An improved dynamic Monte Carlo model coupled with Poisson equation to simulate the performance of organic photovoltaic devices. <i>Journal of Chemical Physics</i> , <b>2011</b> , 134, 124102	3.9	58
66	First-principles investigation of organic semiconductors for thermoelectric applications. <i>Journal of Chemical Physics</i> , <b>2009</b> , 131, 224704	3.9	58
65	GeAs <sub>2</sub> : A IV-V Group Two-Dimensional Semiconductor with Ultralow Thermal Conductivity and High Thermoelectric Efficiency. <i>Chemistry of Materials</i> , <b>2017</b> , 29, 6261-6268	9.6	57
64	Computational evaluation of optoelectronic properties for organic/carbon materials. <i>Accounts of Chemical Research</i> , <b>2014</b> , 47, 3301-9	24.3	54
63	The role of acoustic phonon scattering in charge transport in organic semiconductors: a first-principles deformation-potential study. <i>Science in China Series B: Chemistry</i> , <b>2009</b> , 52, 1646-1652		53
62	Electron-phonon couplings and carrier mobility in graphynes sheet calculated using the Wannier-interpolation approach. <i>Journal of Chemical Physics</i> , <b>2014</b> , 141, 034704	3.9	52
61	Unveiling the Layer-Dependent Catalytic Activity of PtSe Atomic Crystals for the Hydrogen Evolution Reaction. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 6977-6981	16.4	50
60	Layer-Dependent Chemically Induced Phase Transition of Two-Dimensional MoS <sub>2</sub> . <i>Nano Letters</i> , <b>2018</b> , 18, 3435-3440	11.5	50
59	Theoretical insight into the aggregation induced emission phenomena of diphenyldibenzofulvene: a nonadiabatic molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 14207-16	3.6	49
58	First-Principles Predictions of Thermoelectric Figure of Merit for Organic Materials: Deformation Potential Approximation. <i>Journal of Chemical Theory and Computation</i> , <b>2012</b> , 8, 3338-47	6.4	48
57	Hydrogen Bonding-Induced Morphology Dependence of Long-Lived Organic Room-Temperature Phosphorescence: A Computational Study. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 6948-6954	6.4	45

56	Proton transport pathway in the CLC Cl <sup>-</sup> /H <sup>+</sup> antiporter. <i>Biophysical Journal</i> , <b>2009</b> , 97, 121-31	2.9	43
55	Puckered Arsenene: A Promising Room-Temperature Thermoelectric Material from First-Principles Prediction. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 19080-19086	3.8	42
54	Tuning Thermal Transport in Chain-Oriented Conducting Polymers for Enhanced Thermoelectric Efficiency: A Computational Study. <i>Advanced Functional Materials</i> , <b>2017</b> , 27, 1702847	15.6	41
53	Few-quintuple BiTe <sub>2</sub> nanofilms as potential thermoelectric materials. <i>Scientific Reports</i> , <b>2015</b> , 5, 8099	4.9	41
52	Pyrolytic hydrocarbon growth from cyclopentadiene. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 12411-62.8		41
51	Janus monolayer of WSeTe, a new structural phase transition material driven by electrostatic gating. <i>Nanoscale</i> , <b>2018</b> , 10, 21629-21633	7.7	41
50	Molecular dynamics simulations of the supramolecular assembly between an azobenzene-containing surfactant and $\beta$ -cyclodextrin: role of photoisomerization. <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 823-32	3.4	40
49	Anisotropic Thermal Transport in Organic Molecular Crystals from Nonequilibrium Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 5940-5946	3.8	39
48	An ab initio quartic force field of PH <sub>3</sub> . <i>Journal of Chemical Physics</i> , <b>2000</b> , 112, 9624-9631	3.9	39
47	Intrinsic Charge Transport in Stanene: Roles of Bucklings and Electron-Phonon Couplings. <i>Advanced Electronic Materials</i> , <b>2017</b> , 3, 1700143	6.4	38
46	Computational characterization of organic photovoltaic devices. <i>Theoretical Chemistry Accounts</i> , <b>2011</b> , 129, 291-301	1.9	37
45	Single molecule-mediated assembly of polyoxometalate single-cluster rings and their three-dimensional superstructures. <i>Science Advances</i> , <b>2019</b> , 5, eaax1081	14.3	35
44	Communications: A nonperturbative quantum master equation approach to charge carrier transport in organic molecular crystals. <i>Journal of Chemical Physics</i> , <b>2010</b> , 132, 081101	3.9	35
43	Electronic properties and charge carrier mobilities of graphynes and graphdiynes from first principles. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2015</b> , 5, 215-227	7.9	34
42	Doping optimization of organic-inorganic hybrid perovskite CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> for high thermoelectric efficiency. <i>Synthetic Metals</i> , <b>2017</b> , 225, 108-114	3.6	27
41	Suppression of the Charge Density Wave State in Two-Dimensional 1T-TiSe by Atmospheric Oxidation. <i>Angewandte Chemie - International Edition</i> , <b>2017</b> , 56, 8981-8985	16.4	27
40	Unveiling the Layer-Dependent Catalytic Activity of PtSe <sub>2</sub> Atomic Crystals for the Hydrogen Evolution Reaction. <i>Angewandte Chemie</i> , <b>2019</b> , 131, 7051-7055	3.6	27
39	High thermoelectric performance from optimization of hole-doped CuInTe <sub>2</sub> . <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 5925-31	3.6	27

38	Nonadiabatic Molecular Dynamics Modeling of the Intrachain Charge Transport in Conjugated Diketopyrrolo-pyrrole Polymers. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 6631-6640	3.8	26
37	Understanding Lattice Strain-Controlled Charge Transport in Organic Semiconductors: A Computational Study. <i>Advanced Functional Materials</i> , <b>2014</b> , 24, 5531-5540	15.6	25
36	Probing the crystallographic orientation of two-dimensional atomic crystals with supramolecular self-assembly. <i>Nature Communications</i> , <b>2017</b> , 8, 377	17.4	25
35	High-Performance Organic Thermoelectric Materials: Theoretical Insights and Computational Design. <i>Advanced Electronic Materials</i> , <b>2019</b> , 5, 1800882	6.4	24
34	Radical-molecule reactions for aromatic growth: a case study for cyclopentadienyl and acenaphthylene. <i>Journal of Organic Chemistry</i> , <b>2006</b> , 71, 8365-71	4.2	24
33	Aggregation-Induced Emission: A Rising Star in Chemistry and Materials Science. <i>Chinese Journal of Chemistry</i> , <b>2021</b> , 39, 677-689	4.9	24
32	Charge control of fluorescent probes to selectively target the cell membrane or mitochondria: theoretical prediction and experimental validation. <i>Materials Horizons</i> , <b>2019</b> , 6, 2016-2023	14.4	21
31	Coarse-grained molecular dynamics simulations of photoswitchable assembly and disassembly. <i>Nanoscale</i> , <b>2013</b> , 5, 3681-9	7.7	21
30	Lattice thermal conductivity of monolayer AsP from first-principles molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 14024-14030	3.6	20
29	Pressure-induced emission enhancement in hexaphenylsilole: a computational study. <i>Journal of Materials Chemistry C</i> , <b>2019</b> , 7, 1388-1398	7.1	19
28	Device simulation of low-band gap polymer solar cells: Influence of electron-hole pair dissociation and decay rates on open-circuit voltage. <i>Applied Physics Letters</i> , <b>2010</b> , 97, 143511	3.4	17
27	Protein structure and dynamics from single-molecule fluorescence resonance energy transfer. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 1626-34	3.4	17
26	High-resolution Fourier transform spectrum of the (4000) local mode overtone of GeH <sub>4</sub> : local mode effect. <i>Journal of Molecular Structure</i> , <b>2000</b> , 517-518, 41-51	3.4	17
25	Continuous synthesis of carbon dots with full spectrum fluorescence and the mechanism of their multiple color emission. <i>Lab on A Chip</i> , <b>2019</b> , 19, 3974-3978	7.2	16
24	Metal-Free Magnetism in Chemically Doped Covalent Organic Frameworks. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 11013-11021	16.4	15
23	Kinetics-Controlled Amphiphile Self-Assembly Processes. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 1798-1803	6.4	14
22	Substitution effects on the electrical transporting properties of tetrathia[22]annulene[2,1,2,1]: experimental and theoretical investigations. <i>Journal of Materials Chemistry C</i> , <b>2013</b> , 1, 5765	7.1	14
21	Fuller-Rylenes: Cross-Dimensional Molecular Carbons. <i>CCS Chemistry</i> , <b>2020</b> , 2, 271-279	7.2	14

20	Stretching single polymer chains of donor-acceptor foldamers: toward the quantitative study on the extent of folding. <i>Langmuir</i> , <b>2013</b> , 29, 14438-43	4	13
19	High resolution spectroscopic study of CH <sub>3</sub> D in the region 5900-100 cm <sup>-1</sup> . <i>Molecular Physics</i> , <b>1999</b> , 97, 787-795	1.7	13
18	Theoretical Studies on the Deformation Potential, Electron-Phonon Coupling, and Carrier Transports of Layered Systems. <i>Wuli Huaxue Xuebao/Acta Physico - Chimica Sinica</i> , <b>2018</b> , 34, 961-976	3.8	13
17	Anion-binding properties of electron deficient cavities in bis(tetraoxacalix[2]arene[2]triazine): a theoretical study. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 3844-51	2.8	12
16	Reducing Lattice Thermal Conductivity of the Thermoelectric SnSe Monolayer: Role of Phonon-Electron Coupling. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 12001-12006	3.8	11
15	Boosting the Seebeck Coefficient for Organic Coordination Polymers: Role of Doping-Induced Polaron Band Formation. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 2493-2499	6.4	9
14	Self-assembling 1D core/shell microrods by the introduction of additives: a one-pot and shell-tunable method. <i>Chemical Science</i> , <b>2015</b> , 6, 4907-4911	9.4	8
13	Anticancer Polymers via the Biginelli Reaction. <i>ACS Macro Letters</i> , <b>2020</b> , 9, 1249-1254	6.6	8
12	Ferroelectricity in 2D metal phosphorus trichalcogenides and van der Waals heterostructures for photocatalytic water splitting. <i>Journal of Materials Chemistry A</i> , <b>2021</b> , 9, 2734-2741	13	8
11	Efficient fabrication of MoS <sub>2</sub> nanocomposites by water-assisted exfoliation for nonvolatile memories. <i>Green Chemistry</i> , <b>2021</b> , 23, 3642-3648	10	8
10	Nonlinearity of the Dipole Moment Surface and Intensities Anomaly of CHCl <sub>3</sub> . <i>Chinese Physics Letters</i> , <b>2000</b> , 17, 13-15	1.8	7
9	Systematic analysis of reactivities and fragmentation of glutathione and its isomer GluCysGly. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 8222-8	2.8	5
8	High resolution vibration-rotation spectra of the arsine local mode (110 A <sub>1</sub> /E) band. <i>Journal of the Chemical Society, Faraday Transactions</i> , <b>1998</b> , 94, 1397-1401		5
7	High-Resolution Infrared Spectrum of H <sub>3</sub> SiI in the ν <sub>1</sub> /ν <sub>4</sub> Region near 2200 cm <sup>-1</sup> . <i>Journal of Molecular Spectroscopy</i> , <b>1998</b> , 190, 240-7	1.3	4
6	Temperature-Responsive Self-Assembly of Single Polyoxometalates Clusters Driven by Hydrogen Bonds. <i>Advanced Functional Materials</i> , <b>2021</b> , 31, 2103561	15.6	4
5	Understanding the Temperature Dependence of the Seebeck Coefficient from First-Principles Band Structure Calculations for Organic Thermoelectric Materials. <i>CCS Chemistry</i> , <b>2021</b> , 1, 1477-1483	7.2	4
4	Strain induced polymorphism and band structure modulation in low-temperature 2,7-dioctyl[1]benzothieno[3,2-b][1]benzothiophene single crystal. <i>Science China Chemistry</i> , <b>2017</b> , 60, 275-283	7.9	3
3	Janus luminogens with bended intramolecular charge transfer: Toward molecular transistor and brain imaging. <i>Matter</i> , <b>2021</b> ,	12.7	3

2	Coriolis interaction in the local mode ( $n100;F2$ ) combination states of GeH <sub>4</sub> . <i>Molecular Physics</i> , <b>2000</b> , 98, 1409-1413	1.7	2
1	cis-C≡C Bond and Amide Regulated Oriented Supramolecular Assembly on Two-Dimensional Atomic Crystals. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 30996-31002	3.8	1