

Chuan-Lu Yang

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	The molecular structure and spectroscopic properties of C ₃ H ₂ O and its isomers: An ab initio study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 265, 120388.	2.0	4
2	Two-dimensional MgP ₃ monolayer with remarkably tunable bandgap and enhanced visible-light and UV optical absorptions. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 135, 114960.	1.3	26
3	2D XBiSe ₃ (X=Ga, In, Tl) monolayers with high carrier mobility and enhanced visible-light absorption. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 264, 120309.	2.0	7
4	Incorporation of β -aminobutyric acid and cesium cations to formamidinium lead halide perovskites for highly efficient solar cells. <i>Journal of Energy Chemistry</i> , 2022, 64, 561-567.	7.1	19
5	Excellent thermoelectric performances of the SiSe ₂ monolayer and layered bulk. <i>Applied Surface Science</i> , 2022, 575, 151799.	3.1	16
6	First-principles investigations on the feasibility of the GQD-PEB/PUB nanocomposites as the sensitizer of DSSC. <i>Chemical Physics Letters</i> , 2022, 789, 139306.	1.2	3
7	Two-dimensional AlBiX ₃ (X=As, Se, Te) monolayers for photocatalytic water splitting hydrogen evolution reaction under the irradiation of solar light. <i>FlatChem</i> , 2022, 31, 100331.	2.8	3
8	Tunable Dirac states in doping B ₂ S ₃ monolayer. <i>Physical Chemistry Chemical Physics</i> , 2022, , .	1.3	1
9	Z-Scheme photocatalytic solar-energy-to-hydrogen conversion driven by the HfS ₂ /SiSe heterostructure. <i>Journal of Materials Chemistry C</i> , 2022, 10, 5474-5481.	2.7	28
10	Photocatalytic hydrogen evolution reaction with high solar-to-hydrogen efficiency driven by the Sb ₂ S ₃ monolayer and RuI ₂ /Sb ₂ S ₃ heterostructure with solar light. <i>Journal of Power Sources</i> , 2022, 532, 231352.	4.0	40
11	The SiPb monolayer with high thermoelectric performance at room temperature. <i>Surfaces and Interfaces</i> , 2022, 30, 101831.	1.5	1
12	Two-dimensional Sc ₂ CCl ₂ /SiS ₂ van der Waals heterostructure with high solar power conversion efficiency. <i>Applied Surface Science</i> , 2022, 591, 153232.	3.1	8
13	Cesium Copper Iodide Perovskite Nanoscale-Thick Films with Tunable Photoluminescence for White Light-Emitting Diodes. <i>ACS Applied Nano Materials</i> , 2022, 5, 917-924.	2.4	16
14	Modification of SnO ₂ with Phosphorus-Containing Lewis Acid for High-Performance Planar Perovskite Solar Cells with Negligible Hysteresis. <i>Solar Rrl</i> , 2022, 6, .	3.1	17
15	Two-dimensional TeX (X=C, Si, Ge) monolayers with strong intrinsic electric field for efficiency hydrogen evolution reaction. <i>Surfaces and Interfaces</i> , 2022, 31, 102011.	1.5	4
16	Two-dimensional ZnO/BlueP van der Waals heterostructure used for visible-light driven water splitting: A first-principles study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 278, 121359.	2.0	9
17	LiXO ₂ (X=Co, Rh, Ir) and solar light photocatalytic water splitting for hydrogen generation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 279, 121410.	2.0	1
18	Evaluate dimensionless figure of merit for thermoelectric materials based on the intrinsic carrier concentration and bipolar effect. <i>Materials Today Communications</i> , 2022, , 103760.	0.9	0

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19	Effects of the coupling between electrode and QOD-anthoxanthin nanocomposites for dye-sensitized solar cell: DFT and TD-DFT investigations. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 407, 113080.	2.0	16
20	Direct laser cooling the NH molecule with the pseudo-closed loop triplet-triplet transition including intervening electronic states. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 250, 119229.	2.0	4
21	Investigations of the stability and electronic properties of two-dimensional Ga ₂ O ₃ nanosheet in air from first-principles calculations. <i>Applied Surface Science</i> , 2021, 537, 147883.	3.1	14
22	Direct laser cooling schemes for the triatomic SOH and SeOH molecules based on <i>ab initio</i> electronic properties. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2392-2397.	1.3	4
23	The high power conversion efficiency of a two-dimensional GeSe/AsP van der Waals heterostructure for solar energy cells. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6042-6050.	1.3	22
24	Ab initio study of spectroscopic properties at anharmonic force fields of LiNH ₂ . <i>Journal of Molecular Modeling</i> , 2021, 27, 33.	0.8	2
25	Revealing photoluminescence mechanisms of single CsPbBr ₃ /Cs ₄ PbBr ₆ core/shell perovskite nanocrystals. <i>RSC Advances</i> , 2021, 11, 30465-30471.	1.7	4
26	Strain-tunable electronic structure and anisotropic transport properties in Janus MoSSe and g-SiC van der Waals heterostructure. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 9440-9447.	1.3	9
27	Two-dimensional heterostructures of AuSe/SnS for the photocatalytic hydrogen evolution reaction with a Z-scheme. <i>Journal of Materials Chemistry C</i> , 2021, 9, 12231-12238.	2.7	61
28	Thermoelectric performance of BaBiNa and SrBiNa: A first-principle study. <i>Materials Today Communications</i> , 2021, 26, 101971.	0.9	3
29	High thermoelectric efficiency fluoride perovskite materials of AgMF ₃ (M = Zn, Cd). <i>Materials Today Energy</i> , 2021, 19, 100611.	2.5	12
30	Novel 2D B ₂ S ₃ as a metal-free photocatalyst for water splitting. <i>Nanotechnology</i> , 2021, 32, 225401.	1.3	11
31	Imaging of electron transition and bond breaking in the photodissociation of H via ultrafast X-ray photoelectron diffraction. <i>Optics Express</i> , 2021, 29, 10893.	1.7	1
32	Two-dimensional MoSSe/g-GeC van der waals heterostructure as promising multifunctional system for solar energy conversion. <i>Applied Surface Science</i> , 2021, 545, 148952.	3.1	45
33	Ab initio study of spectroscopic properties and anharmonic force fields of MNH ₂ (M = Li, Na, K). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 253, 119591.	2.0	2
34	An alternative indicator of annihilated electrons in atoms: Rahm's electronegativity scale. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2021, 401, 127324.	0.9	1
35	Spectroscopic properties of the low-lying electronic states and laser cooling feasibility for the Srl molecule. <i>Chinese Journal of Physics</i> , 2021, 71, 435-443.	2.0	3
36	Theoretical study on the spectroscopic properties of the low-lying electronic states and the laser cooling feasibility of the Cal molecule. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2021, 270, 107709.	1.1	6

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37	Deep-ultraviolet photodetector based on pulsed-laser-deposited Cs ₃ Cu ₂ I ₅ films/n-Si heterojunction. Optics Letters, 2021, 46, 4252.	1.7	11
38	Halogen Edge-Passivated Antimonene Nanoribbons for Photocatalytic Hydrogen Evolution Reaction with High Solar-to-Hydrogen Conversion. Journal of Physical Chemistry C, 2021, 125, 21341-21351.	1.5	12
39	Newfound two-dimensional Bi ₂ Se ₃ monolayers for driving hydrogen evolution reaction with the visible-light. Applied Surface Science, 2021, 564, 150389.	3.1	7
40	Two-dimensional SiM ₄ (M=Ge, Sn) monolayers as visible-light-driven photocatalyst of hydrogen production. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 261, 120013.	2.0	8
41	First-principles investigation on the thermoelectric performance of half-Heusler compound CuLiX (X=Se, Te). Journal of Physics Condensed Matter, 2021, 33, 095501.	0.7	12
42	First principles study of photoelectrochemical water splitting in monolayer Sn ₂ S ₂ P ₄ with high solar-to-hydrogen efficiency. Applied Physics Letters, 2021, 119, .	1.5	17
43	Luminescence property improvement and controllable color regulation of a novel Bi ³⁺ doped Ca ₂ Ta ₂ O ₇ green phosphor through charge compensation engineering and energy transfer. Physical Chemistry Chemical Physics, 2021, 23, 25886-25895.	1.3	12
44	Two-dimensional BiP ₃ with high carrier mobility and moderate band gap for hydrogen generation from water splitting. Applied Surface Science, 2020, 501, 144263.	3.1	59
45	The spectroscopic properties of the low-lying excited states and laser cooling scheme of SrBr molecule. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 228, 117721.	2.0	4
46	Remarkably High Thermoelectric Efficiencies of the Half-Heusler Compounds BXGa (X = Be, Mg, and Ca). ACS Applied Materials & Interfaces, 2020, 12, 5838-5846.	4.0	39
47	The structures and luminescence properties of Sr ₄ Gd ₃ Na ₃ (PO ₄) ₆ F ₂ :Ce ³⁺ , Tb ³⁺ green phosphors with zero-thermal quenching of Tb ³⁺ for WLEDs. Dalton Transactions, 2020, 49, 667-674.	1.6	34
48	Theoretical study on the low-lying electronic excited states and laser cooling feasibility of AuH molecule. Journal of Quantitative Spectroscopy and Radiative Transfer, 2020, 242, 106770.	1.1	5
49	Remarkable High Thermoelectric Conversion Efficiency Materials of BeMF ₃ (M = Al, Y). Advanced Theory and Simulations, 2020, 3, 2000171.	1.3	9
50	2D XBiSe ₃ (X=As, Sb) monolayers with high anisotropic mobility and enhanced optical absorption in visible light region. Applied Surface Science, 2020, 530, 147137.	3.1	13
51	Surface functional group modification induced partial Fermi level pinning and ohmic contact at borophene-MoS ₂ interfaces. Physical Chemistry Chemical Physics, 2020, 22, 19202-19212.	1.3	4
52	Ab initio study on the molecular structure and spectroscopic properties of isomers of SO ₃ . Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 242, 118746.	2.0	6
53	Modulation in structural and electronic properties of 2D Ga ₂ O ₃ by chemical passivation. Journal of Materials Chemistry C, 2020, 8, 12551-12559.	2.7	13
54	Two-dimensional BP/AsP van der Waals heterostructures as promising photocatalyst for water splitting. Applied Physics Letters, 2020, 117, .	1.5	47

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55	A Single-Molecule and Logic Gate via Optical and Acid-Base Control. <i>Advanced Theory and Simulations</i> , 2020, 3, 2000163.	1.3	7
56	Stereodynamics of the $\text{Ca}^+\text{HCl}^+\text{CaCl}^+\text{H}$ molecular reaction imposed by the rotational excited states of HCl. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26411.	1.0	0
57	Formation of H_3^+ from ethane dication induced by electron impact. <i>Communications Chemistry</i> , 2020, 3, .	2.0	16
58	Insights for vibronic effects on spectral shapes of electronic circular dichroism and circularly polarized luminescence of aza[7]helicene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 239, 118475.	2.0	15
59	Photoluminescence properties and energy transfer of high thermal stable $\text{Na}_2\text{GdPO}_4\text{F}_2\text{:RE}$ (RE = Sm^{3+}). <i>Tj ETQq1 1.0.784314 rgBT /Overlock</i>	1.5	15
60	Gamma-ray spectra in the positron-annihilation process of molecules at room temperature. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020, 384, 126593.	0.9	0
61	Photocatalytic water splitting for hydrogen generation driven by tetragonal, trigonal, hexagonal and cubic LiCoO_2 and visible light. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 239, 118459.	2.0	5
62	Two-dimensional hexaphosphate BiMP_6 (M = Al, Ga, In) with desirable band gaps and ultrahigh carrier mobility for photocatalytic hydrogen evolution. <i>Applied Surface Science</i> , 2020, 517, 146166.	3.1	34
63	SiI_2 monolayer as a promising photocatalyst for water splitting hydrogen production under the irradiation of solar light. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 17517-17524.	3.8	21
64	2D AlP_3 with high carrier mobility and tunable band structure. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 055001.	0.7	19
65	Effects of Adiabatic Approximation on The Electron Momentum Spectroscopy of Partially Spherically Symmetric Molecules. <i>Journal of the Physical Society of Japan</i> , 2020, 89, 074301.	0.7	1
66	Two-dimensional Bi_2Se_3 monolayer with high mobility and enhanced optical absorption in the UV-visible light region. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 124, 114272.	1.3	20
67	Vibrationally resolved electronic circular dichroism and circularly polarized luminescence spectra of a boron-fused double helicene: A theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 231, 118132.	2.0	10
68	ZnCdO_2 monolayer - A complex 2D structure of ZnO and CdO monolayers for photocatalytic water splitting driven by visible-light. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 230, 118068.	2.0	6
69	Ternary chalcogenides XGaS_2 (X = Ag or Cu) for photocatalytic hydrogen generation from water splitting under irradiation of visible light. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26166.	1.0	6
70	High thermoelectric figure of merit and thermopower of HfTe_5 at room temperature. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 345501.	0.7	3
71	Theoretical studies on the feasibility of the hybrid nanocomposites of graphene quantum dot and phenoxazine-based dyes as an efficient sensitizer for dye-sensitized solar cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 206, 216-223.	2.0	23
72	First-principles insight on elastic, electronic, and thermoelectric transport properties of BAgX (X = Ti). <i>Tj ETQq0.0.0 rgBT /Overlock</i>	2.0	12

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73	High mobility and photocatalytic properties of NaXO ₂ (X=Co, Rh, Ir). <i>Vacuum</i> , 2019, 168, 108824.	1.6	7
74	Ascorbic Acid-Assisted Stabilization of Γ -Phase CsPbI ₃ Perovskite for Efficient and Stable Photovoltaic Devices. <i>Solar Rrl</i> , 2019, 3, 1900287.	3.1	25
75	Spectroscopic constants and anharmonic force fields of F ₂ SO: An ab initio study. <i>Chemical Physics Letters</i> , 2019, 736, 136814.	1.2	1
76	Strain effect on the electronic and optical properties of ATaO ₂ N (A=Ca, Sr, and Ba): insights from the first-principles. <i>Applied Physics A: Materials Science and Processing</i> , 2019, 125, 1.	1.1	4
77	Effects of transport direction and carrier concentration on the thermoelectric properties of AgIn ₅ Te ₈ : A first-principles study. <i>Materials Research Bulletin</i> , 2019, 113, 77-83.	2.7	6
78	Anharmonic force fields and spectroscopic constants of H ₂ AsO: An ab initio study. <i>Main Group Chemistry</i> , 2019, 18, 123-137.	0.4	1
79	Spin Logic Gates Operated by Protonation and Magnetism in Molecular Combinational Circuits. <i>Advanced Theory and Simulations</i> , 2019, 2, 1900057.	1.3	8
80	Theoretical insight on the nanocomposite of tetraphenylporphyrin- graphene oxide quantum dot as a sensitizer of DSSC. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 379, 24-31.	2.0	15
81	Theoretical insight into the effect of Si-doped sites on the photocatalytic properties of SrTiO ₃ . <i>Applied Physics A: Materials Science and Processing</i> , 2019, 125, 1.	1.1	4
82	Magnetic field-driven spintronic logic gates in one-dimensional manganese phthalocyanine nanoribbons based molecular spintronic devices. <i>Organic Electronics</i> , 2019, 69, 120-127.	1.4	9
83	Theoretical insight on hybrid nanocomposites of graphene quantum dot and carbazole-carbazole dyes as an efficient sensitizer of DSSC. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 216, 69-75.	2.0	14
84	Pt ₄ cluster catalyzes H ₂ generation from an H ₂ O molecule. <i>Chemical Physics Letters</i> , 2019, 725, 97-101.	1.2	12
85	Effect of M elements (M=Ti, Zr, and Hf) on thermoelectric performance of the half-Heusler compounds MCoBi. <i>Journal Physics D: Applied Physics</i> , 2019, 52, 255501.	1.3	26
86	Mapping of the light-induced conical intersections in the photoelectron spectra of K ₂ molecules. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 207, 348-353.	2.0	3
87	Theoretical study on the low-lying excited electronic states and laser cooling feasibility of CuH molecule. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 212, 55-60.	2.0	5
88	Photocatalytic hydrogen production from water splitting with N-doped $\hat{\Gamma}$ -Ga ₂ O ₃ and visible light. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 211, 71-78.	2.0	23
89	Theoretical insight into the optoelectronic properties of lead-free perovskite derivatives of Cs ₃ Sb ₂ X ₉ (X=Cl, Br, I). <i>Journal of Materials Science</i> , 2019, 54, 4732-4741.	1.7	42
90	Mechanical Tuning of Giant Magnetoresistance and Spin Filtering in Manganese Diporphyrin-Based Molecular Junction. <i>ChemElectroChem</i> , 2019, 6, 421-429.	1.7	1

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91	Quantum interference in the femtosecond photoionization spectra of NaI molecules. <i>Laser Physics Letters</i> , 2019, 16, 016001.	0.6	2
92	Chalcogens doped BaTiO ₃ for visible light photocatalytic hydrogen production from water splitting. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 208, 65-72.	2.0	36
93	O-doped behavior impacts on the optical and mechanical properties of Pmm2-BC2N. <i>Journal of Materials Science</i> , 2019, 54, 457-466.	1.7	5
94	Mechanism of Fluorescence Quenching by Acylamino Twist in the Excited State for 1-(Acylamino)anthraquinones. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2864-2870.	1.1	27
95	OPE molecular junction as a hydrogen gas sensor. <i>Current Applied Physics</i> , 2018, 18, 273-279.	1.1	4
96	Theoretical studies on the possible sensitizers of DSSC: Nanocomposites of graphene quantum dot hybrid phthalocyanine/tetrabenzoporphyrin/tetrabenzotriazaporphyrins/cis-tetrabenzodiazaporphyrins/tetrabenzomonoazaporphyrins and their Cu-metallated macrocycles. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 195, 176-183.		
97	Computational studies on the absorption enhancement of nanocomposites of tetraphenylporphyrin and graphene quantum dot as sensitizers in solar cell. <i>Journal of Materials Science</i> , 2018, 53, 5140-5150.	1.7	14
98	AgKTe: An intrinsic semiconductor material with high thermoelectric properties at room temperature. <i>Journal of Alloys and Compounds</i> , 2018, 739, 35-40.	2.8	14
99	The effect of benzoannulation on intermolecular hydrogen bond and proton transfer of 2-methyl-3-hydroxy-4(1H)quinolone in methanol: A DFT study. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3803.		5
100	Synthesis and Study of Optical Characteristics of TiO ₂ /CdS Hybrid Sphere Structures. <i>Nanoscale Research Letters</i> , 2018, 13, 80.	3.1	2
101	Electronic structure and photoluminescence properties of single component white emitting Sr ₃ LuNa(PO ₄) ₃ F:Eu ²⁺ , Mn ²⁺ phosphor for WLEDs. <i>Journal of Materials Chemistry C</i> , 2018, 6, 4435-4443.	2.7	39
102	Enhancement of the optical absorption of carbon group elements doped ZnS in the visible light range. <i>Renewable Energy</i> , 2018, 117, 22-27.	4.3	30
103	DFT calculations for anharmonic force field and spectroscopic constants of YC ₂ and its ¹³ C isotopologues. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 191, 382-388.	2.0	8
104	The ground and low-lying excited states and feasibility of laser cooling for GaH ⁺ and InH ⁺ cations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 193, 78-86.	2.0	5
105	Efficient green phosphor realized by Ce ³⁺ Tb ³⁺ energy transfer in Li ₃ Sc ₂ (PO ₄) ₃ for ultraviolet white light-emitting diodes. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 26995-27002.	1.3	36
106	Group-IVA element-doped SrIn ₂ O ₄ as potential materials for hydrogen production from water splitting with solar energy. <i>RSC Advances</i> , 2018, 8, 32317-32324.	1.7	0
107	Geometric phase effects on photodissociation dynamics of diatomics. <i>Journal of Chemical Physics</i> , 2018, 149, 224307.	1.2	9
108	Color tunable Ba ₃ Lu(PO ₄) ₃ :Tb ³⁺ , Mn ²⁺ phosphor via Tb ³⁺ Mn ²⁺ energy transfer for white LEDs. <i>Ceramics International</i> , 2018, 44, 15243-15248.	2.3	12

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109	Controlling spin off state by gas molecules adsorption on metal-phthalocyanine molecular junctions and its possibility of gas sensor. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2018, 382, 2666-2672.	0.9	19
110	A theoretical study on the laser cooling scheme for the three-energy-level system of the CN molecule. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2018, 51, 155102.	0.6	3
111	Control of photodissociation of the NaI molecule via pulse chirping. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 20957-20962.	1.3	8
112	Molecular Dynamics Study on Encapsulation of Double Stranded Nucleic Acids into Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2018, 122, 19236-19242.	1.5	2
113	Te-doped perovskite NaTaO ₃ as a promising photocatalytic material for hydrogen production from water splitting driven by visible light. <i>Materials Research Bulletin</i> , 2018, 107, 125-131.	2.7	31
114	Optical absorption enhancement of Hg-doped ZnX (X= S, Se) for hydrogen production from water splitting driven by solar energy. <i>Vacuum</i> , 2018, 157, 36-44.	1.6	5
115	Hydrogen generation from water molecule with Pt ₇ clusters. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 4032-4039.	3.8	19
116	Negative differential resistance and switch behavior of T-B N (x, y= 5, 6, 11) molecular junctions. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2017, 381, 1493-1497.	0.9	1
117	Electronic and optical properties of superhard Ca ²⁺ N materials: a first-principles study. <i>Journal of Computational Electronics</i> , 2017, 16, 262-271.	1.3	4
118	The low-lying electronic states and optical schemes for the laser cooling of the BH ⁺ and BH ²⁺ ions. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 182, 130-135.	2.0	16
119	Cation substitution induced novel gehlenite Ca ₂ GaAlSiO ₇ :Eu ²⁺ /Ce ³⁺ phosphor with green/blue emission for UV-WLEDs. <i>RSC Advances</i> , 2017, 7, 28647-28654.	1.7	16
120	Spectroscopic parameters of the low-lying electronic states and laser cooling feasibility of NH ⁺ cation and NH ²⁺ anion. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 185, 365-370.	2.0	16
121	Constructing sub-10-nm gaps in graphene-metal hybrid system for advanced surface-enhanced Raman scattering detection. <i>Journal of Alloys and Compounds</i> , 2017, 720, 139-146.	2.8	16
122	Reply to "Comment on "Gamma-ray spectra from low-energy positron annihilation processes in molecules". <i>Physical Review A</i> , 2017, 95, .	1.0	0
123	Possibility of gas sensor based on C ₂₀ molecular devices. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2017, 381, 1825-1830.	0.9	10
124	Temperature and Wavelength Dependence of Energy Transfer Process Between Quantized States and Surface States in CdSe Quantum Dots. <i>Nanoscale Research Letters</i> , 2017, 12, 222.	3.1	15
125	The large absorption coefficient and photoconductivity of oP12-FeB ₂ high hard material: A first-principles study. <i>Optik</i> , 2017, 138, 160-165.	1.4	2
126	Adsorption and Dissociation of H ₂ on Cluster Al ₆ N. <i>Journal of Cluster Science</i> , 2017, 28, 1335-1344.	1.7	3

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127	Concerted Mechanisms of Excited-State Proton Intramolecular Transfer for Bis-2,4-(2-benzoxazolyl)-hydroquinone and Its Derivatives. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8217-8226.	1.1	6
128	Symmetry-broken effects on electron momentum spectroscopy caused by adiabatic vibration. <i>Chemical Physics Letters</i> , 2017, 687, 116-124.	1.2	2
129	<i>Ab Initio</i> Studies on Spectroscopic Constants for the HAsO Molecule. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7009-7015.	1.1	7
130	Potential color tunable Sr ₃ LaNa(PO ₄) ₃ F:Eu ²⁺ /Tb ³⁺ /Mn ²⁺ phosphor induced by Eu ²⁺ → Tb ³⁺ and Tb ³⁺ → Mn ²⁺ energy transfer for WLEDs. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 24566-24573.	1.3	15
131	First-principles study on the electronic and optical properties of WS ₂ and MoS ₂ monolayers. <i>Chinese Journal of Physics</i> , 2017, 55, 1930-1937.	2.0	36
132	Quantum reaction dynamics of C(¹ D) + HD → CH(CD) + D(H) on the ground state potential energy surface. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25431.	1.0	6
133	Spin transport properties and spin logic gates in manganese phthalocyanine-based molecular combinational circuits. <i>Journal of Materials Chemistry C</i> , 2017, 5, 8862-8868.	2.7	23
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