Mei-Shan Wang

List of Publications by Year
in descending order

282	3,158	230014	325983
papers	citations	27 h-index	40 g-index

287	287	287	2908
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The molecular structure and spectroscopic properties of C3H2O and its isomers: An ab initio study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 265, 120388.	2.0	4
2	Two-dimensional MgP3 monolayer with remarkably tunable bandgap and enhanced visible-light and UV optical absorptions. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 135, 114960.	1.3	26
3	2D XBiSe3(XÂ=ÂGa, In, Tl) monolayers with high carrier mobility and enhanced visible-light absorption. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 264, 120309.	2.0	7
4	Excellent thermoelectric performances of the SiSe2 monolayer and layered bulk. Applied Surface Science, 2022, 575, 151799.	3.1	16
5	First-principles investigations on the feasibility of the GQD-PEB/PUB nanocomposites as the sensitizer of DSSC. Chemical Physics Letters, 2022, 789, 139306.	1.2	3
6	Impurity Controlled near Infrared Surface Plasmonic in AlN. Nanomaterials, 2022, 12, 459.	1.9	1
7	Two-dimensional AlBiX3(XÂ=ÂS, Se, Te) monolayers for photocatalytic water splitting hydrogen evolution reaction under the irradiation of solar light. FlatChem, 2022, 31, 100331.	2.8	3
8	Assembling of Perylene, Naphthalene, and Pyromellitic Diimide-Based Materials and Their Third-Order Nonlinear Optical Properties. Journal of Physical Chemistry A, 2022, 126, 870-878.	1.1	8
9	Z-Scheme photocatalytic solar-energy-to-hydrogen conversion driven by the HfS₂/SiSe heterostructure. Journal of Materials Chemistry C, 2022, 10, 5474-5481.	2.7	28
10	Control one-dimensional length of rectangular pore on graphene membrane for better desalination performance. Nanotechnology, 2022, 33, 245705.	1.3	4
11	Photocatalytic hydrogen evolution reaction with high solar-to-hydrogen efficiency driven by the Sb2S3 monolayer and RuI2/Sb2S3 heterostructure with solar light. Journal of Power Sources, 2022, 532, 231352.	4.0	40
12	The SiPb monolayer with high thermoelectric performance at room temperature. Surfaces and Interfaces, 2022, 30, 101831.	1.5	1
13	Two-dimensional Sc2CCl2/SiS2 van der Waals heterostructure with high solar power conversion efficiency. Applied Surface Science, 2022, 591, 153232.	3.1	8
14	Theoretical study on some carbohelicenes dyes with tunable emission wavelength: Optical properties, vibronic effect, quantum yield. Dyes and Pigments, 2022, 204, 110407.	2.0	3
15	The effect of intramolecular and intermolecular charge transfers on the third order nonlinear optical properties of the selfâ˜assemble chromophores. Journal of Luminescence, 2022, , 118991.	1.5	1
16	Two-dimensional TeX(X=C, Si, Ge) monolayers with strong intrinsic electric field for efficiency hydrogen evolution reaction. Surfaces and Interfaces, 2022, 31, 102011.	1.5	4
17	Aggregation behavior of partially contacted graphene sheets in six-carbon alkanes: all-atom molecular dynamics simulation. Journal of Molecular Modeling, 2022, 28, .	0.8	1
18	Evaluate dimensionless figure of merit for thermoelectric materials based on the intrinsic carrier concentration and bipolar effect. Materials Today Communications, 2022, , 103760.	0.9	0

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19	Spectroscopic constants and anharmonic force field of dithioformic acid and its isomers: a theoretical study. Journal of Molecular Modeling, 2022, 28, .	0.8	1
20	The spectral-shapes of absorption, emission, ECD and CPL of a fluorene-fused [7]helicene: Vibronic effect and solvent inhomogenous broadening. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 249, 119293.	2.0	3
21	Direct laser cooling the NH molecule with the pseudo-closed loop triplet-triplet transition including intervening electronic states. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 250, 119229.	2.0	4
22	Direct laser cooling schemes for the triatomic SOH and SeOH molecules based on ab initio electronic properties. Physical Chemistry Chemical Physics, 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. Physical Chemistry Chemical Physics, 2021, 23, 6042-6050.	1.3	22
24	Ab initio study of spectroscopic properties at anharmonic force fields of LiNH2. Journal of Molecular Modeling, 2021, 27, 33.	0.8	2
25	Two-dimensional heterostructures of AuSe/SnS for the photocatalytic hydrogen evolution reaction with a Z-scheme. Journal of Materials Chemistry C, 2021, 9, 12231-12238.	2.7	61
26	Thermoelectric performance of BaBiNa and SrBiNa: A first-principle study. Materials Today Communications, 2021, 26, 101971.	0.9	3
27	High thermoelectric efficiency fluoride perovskite materials of AgMF3 (MÂ= Zn, Cd). Materials Today Energy, 2021, 19, 100611.	2.5	12
28	Photophysical investigation of maleimide units substituted [5]carbohelicene derivatives: Absorption, emission, ECD and CPL spectral-shapes. Journal of Luminescence, 2021, 233, 117894.	1.5	3
29	Ab initio study of spectroscopic properties and anharmonic force fields of MNH2 (MÂ=ÂLi, Na, K). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 253, 119591.	2.0	2
30	Spectroscopic properties of the low-lying electronic states and laser cooling feasibility for the SrI molecule. Chinese Journal of Physics, 2021, 71, 435-443.	2.0	3
31	Ultrafast Photoisomerization of N-(2-Methoxybenzylidene)aniline: Nonadiabatic Surface-Hopping Study. Journal of Physical Chemistry A, 2021, 125, 7151-7160.	1.1	2
32	Theoretical study on the spectroscopic properties of the low-lying electronic states and the laser cooling feasibility of the CaI molecule. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 270, 107709.	1.1	6
33	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
34	Newfound two-dimensional Bi2Se3 monolayers for driving hydrogen evolution reaction with the visible-light. Applied Surface Science, 2021, 564, 150389.	3.1	7
35	Rovibrational spectroscopic constants and anharmonic force fields of CH3AsH2 and CH2AsH3: An study. Chemical Physics Letters, 2021, 780, 138917.	1.2	1
36	Vibronic effect explains ECD spectral shape and tunability of CPL wavelength of two triarylborane-based [5]helicenes derivatives. Journal of Luminescence, 2021, 239, 118374.	1.5	6

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37	Two-dimensional SiMI4(MÂ=ÂGe, Sn) monolayers as visible-light-driven photocatalyst of hydrogen production. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 261, 120013.	2.0	8
38	Vibrationally resolved absorption and emission spectral shapes of one 5-carbohelicene derivative: A theoretical study. Chemical Physics Letters, 2021, 783, 139067.	1.2	0
39	First-principles investigation on the thermoelectric performance of half-Heusler compound CuLiX(Xâ€‰=â€‰Se, Te). Journal of Physics Condensed Matter, 2021, 33, 095501.	0.7	12
40	Intra-Molecular Electrical Field Regulated Nonlinear Catalyst Charge Transfer in the Organic Conjugated Molecular System. Catalysts, 2021, 11, 1375.	1.6	0
41	Two-dimensional BiP3 with high carrier mobility and moderate band gap for hydrogen generation from water splitting. Applied Surface Science, 2020, 501, 144263.	3.1	59
42	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
43	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
44	The influence of the isotope substitution on the OÂ+ÂLiH+/LiD+ reactions. Chemical Physics Letters, 2020, 740, 137044.	1.2	2
45	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
46	Remarkable High Thermoelectric Conversion Efficiency Materials of BeMF₃ (M = Al, Y). Advanced Theory and Simulations, 2020, 3, 2000171.	1.3	9
47	2D XBiSe3(XÂ=ÂAs, Sb) monolayers with high anisotropic mobility and enhanced optical absorption in visible light region. Applied Surface Science, 2020, 530, 147137.	3.1	13
48	Ab initio study on the molecular structure and spectroscopic properties of isomers of SO3. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 242, 118746.	2.0	6
49	Insights for vibronic effects on spectral shapes of electronic circular dichroism and circularly polarized luminescence of aza[7]helicene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 239, 118475.	2.0	15
50	Size Dependence of [n]Cycloparaphenylenes (n = 9â€“20): Relationship between Aromaticity and Third-Order Nonlinear Optical Properties. Journal of Physical Chemistry C, 2020, 124, 11081-11091.	1.5	16
51	Photocatalytic water splitting for hydrogen generation driven by tetragonal, trigonal, hexagonal and cubic LiCoO2 and visible light. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 239, 118459.	2.0	5
52	Two-dimensional hexaphosphate BiMP6 (MÂ=ÂAl, Ga, In) with desirable band gaps and ultrahigh carrier mobility for photocatalytic hydrogen evolution. Applied Surface Science, 2020, 517, 146166.	3.1	34
53	SiI2 monolayer as a promising photocatalyst for water splitting hydrogen production under the irradiation of solar light. International Journal of Hydrogen Energy, 2020, 45, 17517-17524.	3.8	21
54	Numerical simulation of temperature field in crack of supercritical carbon dioxide fracturing. Energy Science and Engineering, 2020, 8, 2141-2150.	1.9	6

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55	Rational design of graphene slit as nano check valve. Carbon, 2020, 163, 113-119.	5.4	2
56	Theoretical study of surface-enhanced Raman scattering mechanism of scandium-doped copper/silver clusters. Nanotechnology, 2020, 31, 285201.	1.3	1
57	2D AlP₃ with high carrier mobility and tunable band structure. Journal of Physics Condensed Matter, 2020, 32, 055001.	0.7	19
58	Studies on spectroscopic constants for H2PO and D2PO free radicals. Chemical Physics Letters, 2020, 754, 137750.	1.2	2
59	Two-dimensional Bi2Se3 monolayer with high mobility and enhanced optical absorption in the UVâ€“visible light region. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 124, 114272.	1.3	20
60	Vibrationally resolved electronic circular dichroism and circularly polarized luminescence spectra of a boron-fused double helicene: A theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 231, 118132.	2.0	10
61	ZnCdO2 monolayer â€" A complex 2D structure of ZnO and CdO monolayers for photocatalytic water splitting driven by visible-light. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 230, 118068.	2.0	6
62	Ternary chalcogenides XGaS₂ (X = Ag or Cu) for photocatalytic hydrogen generation from water splitting under irradiation of visible light. International Journal of Quantum Chemistry, 2020, 120, e26166.	1.0	6
63	High thermoelectric figure of merit and thermopower of HfTe₅ at room temperature. Journal of Physics Condensed Matter, 2020, 32, 345501.	0.7	3
64	Theoretical Simulations of Heavy-Atom Kinetic Isotope Effects in Aliphatic Claisen Rearrangement. Journal of Physical Chemistry A, 2020, 124, 10678-10686.	1.1	1
65	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. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 206, 216-223.	2.0	23
66	First-principles insight on elastic, electronic, and thermoelectric transport properties of BAgX (Xâ€¯=â€¯Ti,) Tj ETQq0 0 0 rgBT /Overlock	2.0	12
67	High mobility and photocatalytic properties of NaXO2(X=Co, Rh, Ir). Vacuum, 2019, 168, 108824.	1.6	7
68	Spectroscopic constants and anharmonic force fields of F2SO: An ab inito study. Chemical Physics Letters, 2019, 736, 136814.	1.2	1
69	Strain effect on the electronic and optical properties of ATaO2N (Aâ€‰=â€‰Ca, Sr, and Ba): insights from the first-principles. Applied Physics A: Materials Science and Processing, 2019, 125, 1.	1.1	4
70	Effects of transport direction and carrier concentration on the thermoelectric properties of AgIn5Te8: A first-principles study. Materials Research Bulletin, 2019, 113, 77-83.	2.7	6
71	Anharmonic force fields and spectroscopic constants of H2AsO: An ab initio study. Main Group Chemistry, 2019, 18, 123-137.	0.4	1
72	Theoretical insight on the nanocomposite of tetraphenylporphyrin- graphene oxide quantum dot as a sensitizer of DSSC. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 379, 24-31.	2.0	15

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73	Theoretical insight into the effect of Si-doped sites on the photocatalytic properties of SrTiO3. Applied Physics A: Materials Science and Processing, 2019, 125, 1.	1.1	4
74	Theoretical insight on hybrid nanocomposites of graphene quantum dot and carbazoleâ€“carbazole dyes as an efficient sensitizer of DSSC. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 216, 69-75.	2.0	14
75	Pt4 cluster catalyzes H2 generation from an H2O molecule. Chemical Physics Letters, 2019, 725, 97-101.	1.2	12
76	Effect of M elements (Mâ€‰â€‰=â€‰â€‰Ti, Zr, and Hf) on thermoelectric performance of the half-Heusler compounds MCoBi. Journal Physics D: Applied Physics, 2019, 52, 255501.	1.3	26
77	Volume-conserving photoisomerization of a nonplanar GFP chromophore derivative: Nonadiabatic dynamics simulation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 214, 86-94.	2.0	2
78	Lateral scaling and positioning effects of top-gate electrodes on single-molecule field-effect transistors. Journal of Physics Condensed Matter, 2019, 31, 285302.	0.7	2
79	Theoretical study on the low-lying excited electronic states and laser cooling feasibility of CuH molecule. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 212, 55-60.	2.0	5
80	Photocatalytic hydrogen production from water splitting with N-doped Î²-Ga2O3 and visible light. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 211, 71-78.	2.0	23
81	Theoretical insight into the optoelectronic properties of lead-free perovskite derivatives of Cs3Sb2X9 (Xâ€‰=â€‰Cl, Br, I). Journal of Materials Science, 2019, 54, 4732-4741.	1.7	42
82	A new potential energy surface of the LiHO+ system and the dynamics studies of the Oâ€¯+â€¯LiH+ reaction. Chemical Physics Letters, 2019, 715, 123-128.	1.2	2
83	Chalcogens doped BaTiO3 for visible light photocatalytic hydrogen production from water splitting. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 208, 65-72.	2.0	36
84	O-doped behavior impacts on the optical and mechanical properties of Pmm2-BC2N. Journal of Materials Science, 2019, 54, 457-466.	1.7	5
85	Mechanism of Fluorescence Quenching by Acylamino Twist in the Excited State for 1-(Acylamino)anthraquinones. Journal of Physical Chemistry A, 2018, 122, 2864-2870.	1.1	27
86	OPE molecular junction as a hydrogen gas sensor. Current Applied Physics, 2018, 18, 273-279.	1.1	4
87	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. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 195, 176-183.	2.0	19
88	Computational studies on the absorption enhancement of nanocomposites of tetraphenylporphyrin and graphene quantum dot as sensitizers in solar cell. Journal of Materials Science, 2018, 53, 5140-5150.	1.7	14
89	AgKTe: An intrinsic semiconductor material with high thermoelectric properties at room temperature. Journal of Alloys and Compounds, 2018, 739, 35-40.	2.8	14
90	The effect of benzoâ€annelation on intermolecular hydrogen bond and proton transfer of 2â€methylâ€3â€hydroxyâ€4(<scp>1H</scp>)â€quinolone in methanol: A <scp>TDâ€DFT</scp> study. Journal of Physical Organic Chemistry, 2018, 31, e3803.	1.9	5

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91	Enhancement of the optical absorption of carbon group elements doped ZnS in the visible light range. Renewable Energy, 2018, 117, 22-27.	4.3	30
92	Nonadiabatic dynamics simulation of photoisomerization mechanism of the second stablest isomer of N-salicilydenemethylfurylamine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 191, 315-324.	2.0	7
93	DFT calculations for anharmonic force field and spectroscopic constants of YC2 and its 13C isotopologues. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 191, 382-388.	2.0	8
94	The ground and low-lying excited states and feasibility of laser cooling for GaH+ and InH+ cations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 193, 78-86.	2.0	5
95	Group-IVA element-doped SrIn2O4 as potential materials for hydrogen production from water splitting with solar energy. RSC Advances, 2018, 8, 32317-32324.	1.7	0
96	The theoretical study of the ground and excited states properties for F2BO and H2BO free radicals. AIP Advances, 2018, 8, 055021.	0.6	1
97	Constructing Sensitive and Fast Lead-Free Single-Crystalline Perovskite Photodetectors. Journal of Physical Chemistry Letters, 2018, 9, 3087-3092.	2.1	92
98	A theoretical study on the laser cooling scheme for the three-energy-level system of the CN molecule. Journal of Physics B: Atomic, Molecular and Optical Physics, 2018, 51, 155102.	0.6	3
99	Te-doped perovskite NaTaO3 as a promising photocatalytic material for hydrogen production from water splitting driven by visible light. Materials Research Bulletin, 2018, 107, 125-131.	2.7	31
100	The ketoâ†'enol photoisomerization of Nâ€salicilydenemethylfurylamine: Nonadiabatic ab initio dynamics simulation. International Journal of Quantum Chemistry, 2018, 118, e25656.	1.0	1
101	Ultrafasttrans-cisphotoisomerization of the neutral chromophore in green fluorescent proteins: Surface-hopping dynamics simulation. Journal of Chemical Physics, 2018, 149, 074304.	1.2	4
102	Optical absorption enhancement of Hg-doped ZnX (X= S, Se) for hydrogen production from water splitting driven by solar energy. Vacuum, 2018, 157, 36-44.	1.6	5
103	Hydrogen generation from water molecule with Pt7 clusters. International Journal of Hydrogen Energy, 2017, 42, 4032-4039.	3.8	19
104	Negative differential resistance and switch behavior of T-B N (x, y= 5, 6, 11) molecular junctions. Physics Letters, Section A: General, Atomic and Solid State Physics, 2017, 381, 1493-1497.	0.9	1
105	Electronic and optical properties of superhard Câ€"N materials: a first-principles study. Journal of Computational Electronics, 2017, 16, 262-271.	1.3	4
106	The low-lying electronic states and optical schemes for the laser cooling of the BH + and BH â^' ions. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 182, 130-135.	2.0	16
107	Spectroscopic parameters of the low-lying electronic states and laser cooling feasibility of NH + cation and NH â^' anion. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 185, 365-370.	2.0	16
108	Constructing sub-10-nm gaps in graphene-metal hybrid system for advanced surface-enhanced Raman scattering detection. Journal of Alloys and Compounds, 2017, 720, 139-146.	2.8	16

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109	Nonadiabaticab initiomolecular dynamics study of photoisomerization inN-salicilydenemethylfurylamine (SMFA). Journal of Chemical Physics, 2017, 146, 124312.	1.2	13
110	Reply to â€œComment on â€˜Gamma-ray spectra from low-energy positron annihilation processes in moleculesâ€™ â€• Physical Review A, 2017, 95, .	1.0	0
111	The large absorption coefficient and photoconductivity of oP12-FeB2 high hard material: A first-principles study. Optik, 2017, 138, 160-165.	1.4	2
112	Adsorption and Dissociation of H2 on Cluster Al6N. Journal of Cluster Science, 2017, 28, 1335-1344.	1.7	3
113	Concerted Mechanisms of Excited-State Proton Intramolecular Transfer for Bis-2,4-(2-benzoxazolyl)-hydroquinone and Its Derivatives. Journal of Physical Chemistry A, 2017, 121, 8217-8226.	1.1	6
114	Symmetry-broken effects on electron momentum spectroscopy caused by adiabatic vibration. Chemical Physics Letters, 2017, 687, 116-124.	1.2	2
115	Ab Initio Studies on Spectroscopic Constants for the HAsO Molecule. Journal of Physical Chemistry A, 2017, 121, 7009-7015.	1.1	7
116	First-principles study on the electronic and optical properties of WS2 and MoS2 monolayers. Chinese Journal of Physics, 2017, 55, 1930-1937.	2.0	36
117	Effect of Ti doping on mechanical and optical properties of super-hard I2d-CN2 materials. RSC Advances, 2017, 7, 37943-37951.	1.7	3
118	Computational anharmonic force fields of CuSH and CuSD. Journal of Physics B: Atomic, Molecular and Optical Physics, 2017, 50, 155102.	0.6	5
119	Structural, Electronic, and Optical Properties of Superhard Materials tP10-FeB4 and I4 1 /acd-FeB4. Journal of Electronic Materials, 2017, 46, 2506-2511.	1.0	1
120	Enhanced photocatalytic performance of anatase TiO 2 substitutionally co-doped with La and N. Solar Energy Materials and Solar Cells, 2017, 170, 233-238.	3.0	12
121	Pristine and Se-/In-doped TlAsS2 enhance the solar energy-driven water splitting for hydrogen generation. International Journal of Hydrogen Energy, 2017, 42, 15464-15470.	3.8	12
122	Theoretical research on bandgap of H-saturated Ga1â^'xAlxN nanowires. International Journal of Modern Physics B, 2017, 31, 1650252.	1.0	4
123	Gamma-ray spectra from low-energy positron annihilation processes in molecules. Physical Review A, 2016, 94, .	1.0	3
124	The spectroscopic constants and anharmonic force field of AgSH: An ab initio study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 164, 89-92.	2.0	6
125	Generating H2 from a H2O molecule by catalysis using a small Al6Cu cluster. Energy, 2016, 106, 131-136.	4.5	26
126	Effects of collision energy on the stereodynamics of the reaction O + H2+â†' OH + H+. Chemical Physics, 2016, 472, 156-162.	0.9	2

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127	Near-infrared photocathode In0.53Ga0.47As doped with zinc: A first principle study. Optik, 2016, 127, 1268-1271.	1.4	4
128	Uniaxial strain effects on the optoelectronic properties of GaN nanowires. Superlattices and Microstructures, 2016, 97, 327-334.	1.4	25
129	Study of Cs adsorption on (100) surface of [001]-oriented GaN nanowires: A first principle research. Applied Surface Science, 2016, 387, 1110-1115.	3.1	46
130	Theoretical study for heterojunction surface of NEA GaN photocathode dispensed with Cs activation. Modern Physics Letters B, 2016, 30, 1650339.	1.0	3
131	Extraction of H2 from H2O molecule using a small Al6Si cluster. International Journal of Hydrogen Energy, 2016, 41, 17858-17863.	3.8	25
132	A first-principles study of the effects of different Al constituents on Ga1â^'xAlxN nanowires. International Journal of Modern Physics B, 2016, 30, 1650217.	1.0	3
133	Enhancement of absorption and conductivity of CdS in the infrared range with Cu dopant. Materials Chemistry and Physics, 2016, 183, 349-355.	2.0	12
134	First-principle study on electronic structure and optical properties of GaN nanowires with different cross-sections. International Journal of Modern Physics B, 2016, 30, 1650136.	1.0	3
135	Research on optoelectronic properties of GaN nanowires with N vacancy. Computational and Theoretical Chemistry, 2016, 1092, 19-24.	1.1	5
136	Low Threshold Two-Photon-Pumped Amplified Spontaneous Emission in CH₃NH₃PbBr₃ Microdisks. ACS Applied Materials & Interfaces, 2016, 8, 19587-19592.	4.0	54
137	Optoelectronic properties of Mg doping GaN nanowires. Optical and Quantum Electronics, 2016, 48, 1.	1.5	5
138	Ab initio studies on the spin-forbidden cooling transitions of the LiRb molecule. Physical Chemistry Chemical Physics, 2016, 18, 19838-19846.	1.3	23
139	Influence of Zn doping on the early activation stage of GaAlAs photocathodes: A density functional theory research. Optik, 2016, 127, 3065-3068.	1.4	1
140	Electron affinity of GaN(0001) surface doped with Al, Mg. Optik, 2016, 127, 3624-3628.	1.4	4
141	Analytic functions for potential energy curves, dipole moments, and transition dipole moments of LiRb molecule. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 153, 488-495.	2.0	8
142	Theoretical study on stereodynamics of H + NeH ⁺ (v=0, j=0) &#8594 NeH ⁺ +H reaction. The Journal of Atomic and Molecular Sciences, 2016, 7, 104-114.	0.1	2
143	Theoretical investigation of the laser cooling of a LiBe molecule. Physical Review A, 2015, 92, .	1.0	31
144	Cesium, oxygen coadsorption on AlGaN(0001) surface: experimental research and ab initio calculations. Journal of Materials Science: Materials in Electronics, 2015, 26, 2181-2188.	1.1	6

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145	Theoretical study of cesium and oxygen activation processes on GaN (0001) surface. Materials Science in Semiconductor Processing, 2015, 39, 61-66.	1.9	10
146	Cesium adsorption on In0.53Ga0.47As (100) Î²2 (2Ã—4) surface: A first-principles research. Applied Surface Science, 2015, 324, 547-553.	3.1	6
147	A DFT study of atomic geometry and electronic structures for oxidized Al0.25Ga0.75N (001) (2Ã—2) reconstruction surfaces. Applied Surface Science, 2015, 333, 201-206.	3.1	7
148	Optical properties of Ga0.75Al0.25N with interstitial defects. Optik, 2015, 126, 3349-3352.	1.4	2
149	Novel optical properties of Î³-Si3N4 with B dopant. Materials Chemistry and Physics, 2015, 161, 170-174.	2.0	1
150	Theoretical investigation of adsorption and dissociation of H2 on cluster Al6Si. International Journal of Hydrogen Energy, 2015, 40, 8911-8916.	3.8	23
151	Electronic structure and optical properties of bulk In0.53Ga0.47As for near-infrared photocathode. Optik, 2015, 126, 1061-1065.	1.4	3
152	Atomic geometry and electronic structures of Be-doped and Be-, O-codoped Ga0.75Al0.25N. Computational Materials Science, 2015, 99, 306-315.	1.4	8
153	Theoretical study of spectroscopic constants and anharmonic force field of SiF2. Journal of Molecular Modeling, 2015, 21, 108.	0.8	8
154	Electronic transport properties of tetracyclopentadienyl modified with C and Si atoms. Physics Letters, Section A: General, Atomic and Solid State Physics, 2015, 379, 1726-1731.	0.9	2
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