Mei-Shan Wang

List of Publications by Year
in descending order

282	3,158	201674 27	289244 40
papers	citations	h-index	g-index

287	287	287	2569
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Crystallization of alkane melts induced by carbon nanotubes and graphene nanosheets: a molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2011, 13, 15476.	2.8	99
2	Constructing Sensitive and Fast Lead-Free Single-Crystalline Perovskite Photodetectors. Journal of Physical Chemistry Letters, 2018, 9, 3087-3092.	4.6	92
3	Interactions between Single-Walled Carbon Nanotubes and Polyethylene/Polypropylene/Polystyrene/Poly(phenylacetylene)/Poly(p-phenylenevinylene) Considering Repeat Unit Arrangements and Conformations:â€‰ A Molecular Dynamics Simulation Study. Journal of Physical Chemistry C, 2008, 112, 1803-1811.	3.1	76
4	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.	5.5	61
5	Two-dimensional BiP3 with high carrier mobility and moderate band gap for hydrogen generation from water splitting. Applied Surface Science, 2020, 501, 144263.	6.1	59
6	First-principles study of structure and quantum transport properties of C20 fullerene. Journal of Chemical Physics, 2009, 131, 024311.	3.0	56
7	First-principles study of transport properties of endohedral Li@C20 metallofullerene. Current Applied Physics, 2010, 10, 260-265.	2.4	56
8	Theoretical study of Cs adsorption on GaN(0001) surface. Applied Surface Science, 2012, 258, 7425-7429.	6.1	54
9	Low Threshold Two-Photon-Pumped Amplified Spontaneous Emission in CH₃NH₃PbBr₃ Microdisks. ACS Applied Materials & Interfaces, 2016, 8, 19587-19592.	8.0	54
10	Attosecond resolution quantum dynamics between electrons andH2+molecules. Physical Review A, 2006, 74, .	2.5	50
11	The stereodynamics of the two reactions: H + LiH+(v = 0, j = 0) â†’ H2 + Li+ and H+ + LiH(v = 0, j = 0) â†’ H2+ + Li. Physical Chemistry Chemical Physics, 2009, 11, 10438.	2.8	47
12	Study of Cs adsorption on (100) surface of [001]-oriented GaN nanowires: A first principle research. Applied Surface Science, 2016, 387, 1110-1115.	6.1	46
13	The novel optical properties of CdS caused by concentration of impurity Co. Journal of Alloys and Compounds, 2014, 585, 503-509.	5.5	45
14	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.	3.7	42
15	Electronic structure and optical properties of zinc-blende GaN. Optik, 2012, 123, 2208-2212.	2.9	40
16	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.	7.8	40
17	Remarkably High Thermoelectric Efficiencies of the Half-Heusler Compounds BXGa (X = Be, Mg, and Ca). ACS Applied Materials & Interfaces, 2020, 12, 5838-5846.	8.0	39
18	First-principles study on the electronic and optical properties of WS2 and MoS2 monolayers. Chinese Journal of Physics, 2017, 55, 1930-1937.	3.9	36

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19	Chalcogens doped BaTiO3 for visible light photocatalytic hydrogen production from water splitting. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 208, 65-72.	3.9	36
20	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.	6.1	34
21	Study of Cs adsorption on Ga(Mg)0.75Al0.25N (0001) surface: A first principle calculation. Applied Surface Science, 2013, 282, 308-314.	6.1	31
22	Theoretical investigation of the laser cooling of a LiBe molecule. Physical Review A, 2015, 92, .	2.5	31
23	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.	5.2	31
24	Enhancement of the optical absorption of carbon group elements doped ZnS in the visible light range. Renewable Energy, 2018, 117, 22-27.	8.9	30
25	Geometrical and Electronic Properties of the Clusters of C20 Cage Doped with Alkali Metal Atoms. Journal of Cluster Science, 2011, 22, 31-39.	3.3	29
26	Effect of functionalization on the interfacial binding energy of carbon nanotube/nylon 6 nanocomposites: a molecular dynamics study. RSC Advances, 2012, 2, 2836.	3.6	29
27	Comparison of optical properties between Wurtzite and zinc-blende Ga0.75Al0.25N. Optik, 2014, 125, 424-427.	2.9	29
28	Z-Scheme photocatalytic solar-energy-to-hydrogen conversion driven by the HfS₂/SiSe heterostructure. Journal of Materials Chemistry C, 2022, 10, 5474-5481.	5.5	28
29	First-Principles Study of Electronic Transport Properties of Dodecahedrane C20H20 and Its Endohedral Complex Li@C20H20. Journal of Physical Chemistry C, 2009, 113, 15756-15760.	3.1	27
30	Mechanism of Fluorescence Quenching by Acylamino Twist in the Excited State for 1-(Acylamino)anthraquinones. Journal of Physical Chemistry A, 2018, 122, 2864-2870.	2.5	27
31	Generating H2 from a H2O molecule by catalysis using a small Al6Cu cluster. Energy, 2016, 106, 131-136.	8.8	26
32	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.	2.8	26
33	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.	2.7	26
34	Uniaxial strain effects on the optoelectronic properties of GaN nanowires. Superlattices and Microstructures, 2016, 97, 327-334.	3.1	25
35	Extraction of H2 from H2O molecule using a small Al6Si cluster. International Journal of Hydrogen Energy, 2016, 41, 17858-17863.	7.1	25
36	DFT/TDDFT study on the excited-state hydrogen bonding dynamics of hydrogen-bonded complex formed by methyl cyanide and methanol. Computational and Theoretical Chemistry, 2011, 964, 243-247.	2.5	24

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37	Quasi-classical trajectory study of the cross sections of the reactions Dâ˜+H2â†'Hâ˜+HD and Hâ˜+D2â†'Dâ˜+HD. Chemical Physics Letters, 2007, 445, 125-128.	2.6	23
38	Theoretical investigation of adsorption and dissociation of H2 on cluster Al6Si. International Journal of Hydrogen Energy, 2015, 40, 8911-8916.	7.1	23
39	Ab initio studies on the spin-forbidden cooling transitions of the LiRb molecule. Physical Chemistry Chemical Physics, 2016, 18, 19838-19846.	2.8	23
40	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.	3.9	23
41	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.	3.9	23
42	Research on electronic structure and optical properties of Mg doped Ga0.75Al0.25N. Optical Materials, 2014, 36, 787-796.	3.6	22
43	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.	2.8	22
44	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.	7.1	21
45	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.	2.7	20
46	Hydrogen generation from water molecule with Pt7 clusters. International Journal of Hydrogen Energy, 2017, 42, 4032-4039.	7.1	19
47	2D AlP₃ with high carrier mobility and tunable band structure. Journal of Physics Condensed Matter, 2020, 32, 055001.	1.8	19
48	Study on the electron structure and optical properties of Ga0.5Al0.5As(100) Î²2(2Ã—4) reconstruction surface. Applied Surface Science, 2013, 266, 380-385.	6.1	18
49	Controllable low-bias negative differential resistance, switching, and rectifying behaviors of dipyrimidinylâ€“diphenyl induced by contact mode. Physica B: Condensed Matter, 2014, 434, 32-37.	2.7	18
50	A comparison of the stereodynamics between the reactions H+HH(D, T) and the reactions Hâ˜+HH(D, T). Chemical Physics, 2008, 348, 97-102.	1.9	17
51	Quasi-classical Trajectory Study of the Ne + H₂⁺ â†' NeH⁺ + H Reaction Based on Global Potential Energy Surface. Journal of Physical Chemistry A, 2011, 115, 1486-1492.	2.5	17
52	Isotopic effects on stereodynamics for the two reactions: H + LiH+(v = 0, j = 0) â†' H2 + Li+ and H+ + LiH(v) Tj ETQq0 0 0 rgBT /Overlock	2.8	16
53	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.	3.9	16
54	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.	3.9	16

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55	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.	5.5	16
56	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.	3.1	16
57	Excellent thermoelectric performances of the SiSe2 monolayer and layered bulk. Applied Surface Science, 2022, 575, 151799.	6.1	16
58	Density Functional Theory Studies of Au_n⁺(CH₃OH)_m (n = 3, 5, m) Tj ETQq0 0 0 rgBT /Overlo	2.3	16
59	Electronic promotion effect of double proton transfer on conduction of DNA through improvement of transverse electronic communication of base pairs. Journal of Chemical Physics, 2011, 135, 134315.	3.0	15
60	The adsorption of Cs and residual gases on Ga0.5Al0.5As (001) Î²2 (2Ã—4) surface: A first principles research. Applied Surface Science, 2014, 290, 142-147.	6.1	15
61	Atomic geometry and electronic structure of Al0.25Ga0.75N(0001) surfaces covered with different coverages of cesium: A first-principle research. Applied Surface Science, 2015, 326, 251-256.	6.1	15
62	Research on Cs activation mechanism for Ga0.5Al0.5As(001) and GaN(0001) surface. Applied Surface Science, 2015, 324, 300-303.	6.1	15
63	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.	3.9	15
64	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.	3.9	15
65	Theoretical characteristics of the bound states of M-X complexes (M=Cu, Ag, and Au, and X=He, Ne, and) Tj ETQq1 1 0.784314 rgBT /O	3.0	14
66	Stereodynamics of the reactions Ne+H⁺₂/Ne+D⁺₂/Ne+T₂. Chinese Physics B, 2012, 21, 043101.	1.4	14
67	Geometry and electronic structure of the Zn-doped GaAs (100) Î²2(2Ã—4) surface: A first-principle study. Applied Surface Science, 2013, 283, 954-957.	6.1	14
68	Enhancing the visible-light absorption of TiO2 with the use of key N, Co, and Na dopant concentrations. Solar Energy Materials and Solar Cells, 2015, 132, 94-100.	6.2	14
69	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.	3.7	14
70	AgKTe: An intrinsic semiconductor material with high thermoelectric properties at room temperature. Journal of Alloys and Compounds, 2018, 739, 35-40.	5.5	14
71	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.	3.9	14
72	An ab initio study of the ground and low-lying excited states of KBe with the effect of inner-shell electrons. Journal of Chemical Physics, 2013, 139, 074305.	3.0	13

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73	Optoelectronic properties of GaN, AlN, and GaAlN alloys. Optik, 2015, 126, 3357-3361.	2.9	13
74	Nonadiabaticab initiomolecular dynamics study of photoisomerization inN-salicilydenemethylfurylamine (SMFA). Journal of Chemical Physics, 2017, 146, 124312.	3.0	13
75	2D XBiSe3(XÂ=ÂAs, Sb) monolayers with high anisotropic mobility and enhanced optical absorption in visible light region. Applied Surface Science, 2020, 530, 147137.	6.1	13
76	Ab initio study of spectroscopic constants and anharmonic force field of Ge74Cl2. Journal of Chemical Physics, 2007, 126, 194301.	3.0	12
77	Cs adsorption on Ga0.5Al0.5As(001)Î²2 (2Ã—4) surface: A first-principles research. Computational Materials Science, 2014, 84, 226-231.	3.0	12
78	Enhancement of absorption and conductivity of CdS in the infrared range with Cu dopant. Materials Chemistry and Physics, 2016, 183, 349-355.	4.0	12
79	Enhanced photocatalytic performance of anatase TiO 2 substitutionally co-doped with La and N. Solar Energy Materials and Solar Cells, 2017, 170, 233-238.	6.2	12
80	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.	7.1	12
81	First-principles insight on elastic, electronic, and thermoelectric transport properties of BAgX (Xâ€¯=â€¯Ti,) Tj ETQq1 1 0.784314 rgBT	4.1	12
82	Pt4 cluster catalyzes H2 generation from an H2O molecule. Chemical Physics Letters, 2019, 725, 97-101.	2.6	12
83	High thermoelectric efficiency fluoride perovskite materials of AgMF3 (MÂ= Zn, Cd). Materials Today Energy, 2021, 19, 100611.	4.7	12
84	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.	3.1	12
85	First-principles investigation on the thermoelectric performance of half-Heusler compound CuLiX(Xâ€‰=â€‰Se, Te). Journal of Physics Condensed Matter, 2021, 33, 095501.	1.8	12
86	Structural, Electronic, and Magnetic Properties of Fe3C2 Cluster. Journal of Physical Chemistry A, 2008, 112, 4556-4561.	2.5	11
87	Theoretical characters of the ground states of YbX (X=F, Cl, Br, I, At). Chemical Physics Letters, 2009, 467, 265-269.	2.6	11
88	Effect of doping Fe and Si on electronic structure and optical Properties of CdS. Physica B: Condensed Matter, 2013, 417, 17-23.	2.7	11
89	First principles calculations of the electronic structure and optical properties of (001), (011) and (111) Ga0.5Al0.5As surfaces. Materials Science in Semiconductor Processing, 2013, 16, 1813-1820.	4.0	11
90	Electronic structure and optical properties of Al and Mg co-doped GaN. Chinese Physics B, 2013, 22, 117103.	1.4	11

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91	Construction of analytic functions for the potential energy curves, dipole moments, and transition dipole moments of RbBe and CsBe molecules. Journal of Quantitative Spectroscopy and Radiative Transfer, 2015, 165, 56-67.	2.3	11
92	Theoretical calculation of the integral cross-sections of the reaction Hâ^'â€‰+â€‰H2â€‰â†'â€‰H2â€‰+â€‰Hâ€‰â^'and its isoto variants. Molecular Physics, 2007, 105, 2329-2333.	1.7	10
93	Dominant role of the interstitial 4d transition-metal in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" display="inline" overflow="scroll"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>TM@Zr</mml:mtext></mml:mrow><mml:mrow><mml:mr (TM = Yâ€“Cd, Z= 0, Â±1) icosahedral cages. Chemical Physics Letters, 2008, 457, 49-53.	2.6	10
94	Ground and low-lying excited states of SO2 studied by the SAC/SAC-CI method. Computational and Theoretical Chemistry, 2008, 859, 7-10.	1.5	10
95	Excited-state hydrogen bonding dynamics of methyl isocyanide in methanol solvent: A DFT/TDDFT study. Open Physics, 2011, 9, .	1.7	10
96	Collision Energies Effect on Stereodynamics for Ne + H ⁺ ₂ â†' NeH ⁺ + H Reaction. Chinese Physics Letters, 2011, 28, 013101.	3.3	10
97	Interactions of Mzâ€“X complexes (M = Cu, Ag, and Au; X = He, Ne, and Ar; and z = Â±1). Journal of Chemical Physics, 2011, 134, 024306.	3.0	10
98	Analytical potential energy functions and spectroscopic properties for the ground and low-lying excited states of KRb. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 99, 57-61.	3.9	10
99	Dynamic mechanism of HIV replication inhibitor peptide encapsulated into carbon nanotubes. Current Applied Physics, 2013, 13, 1001-1007.	2.4	10
100	Theoretical study of cesium and oxygen activation processes on GaN (0001) surface. Materials Science in Semiconductor Processing, 2015, 39, 61-66.	4.0	10
101	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.	2.9	10
102	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.	3.9	10
103	The structure elucidation of a new bromophenol metabolite from Polysiphonia urceolata by experimental and DFT theoretical methods. Journal of Molecular Structure, 2009, 929, 1-5.	3.6	9
104	Orientation effect on the electronic transport properties of C24 fullerene molecule. Physica B: Condensed Matter, 2012, 407, 2247-2253.	2.7	9
105	First principles study on the influence of vacancy defects on electronic structure and optical properties of Ga0.5Al0.5As photocathodes. Optik, 2014, 125, 587-592.	2.9	9
106	Theoretical study on electronic and optical properties of In0.53Ga0.47As (100) Î²2 (2Ã—4) surface. Applied Surface Science, 2014, 288, 238-243.	6.1	9
107	Remarkable High Thermoelectric Conversion Efficiency Materials of BeMF₃ (M = Al, Y). Advanced Theory and Simulations, 2020, 3, 2000171.	2.8	9
108	Isotopic effects on the stereodynamics for the reactions. Chemical Physics, 2011, 379, 46-50.	1.9	8

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109	The geometric structure and electronic properties of Fe3O3+ clusters. Physica B: Condensed Matter, 2011, 406, 200-204.	2.7	8
110	Influence of the reagent vibration on the stereo-dynamics of the reactions D ^{â^'} + H ₂ and H ^{â^'} + D ₂. Chinese Physics B, 2012, 21, 023402.	1.4	8
111	Isothermal Crystallization of Short Polymer Chains Induced by the Oriented Slab and the Stretched Bundle of Polymer: A Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2012, 116, 2040-2047.	2.6	8
112	Quasi-Classical Trajectory Study of the N(2D) + H2(X1Î£G+) â†' NH(X3Î£â€“) + H(2S) Reaction Based on an Analytical Potential Energy Surface. Journal of Physical Chemistry A, 2013, 117, 3-8.	2.5	8
113	Effects of silica surface on the ordered orientation of polyethylene: A molecular dynamics study. Applied Surface Science, 2014, 311, 273-278.	6.1	8
114	Atomic geometry and electronic structures of Be-doped and Be-, O-codoped Ga0.75Al0.25N. Computational Materials Science, 2015, 99, 306-315.	3.0	8
115	Theoretical study of spectroscopic constants and anharmonic force field of SiF2. Journal of Molecular Modeling, 2015, 21, 108.	1.8	8
116	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.	3.9	8
117	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.	3.9	8
118	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.	3.9	8
119	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.	2.5	8
120	Two-dimensional Sc2CCl2/SiS2 van der Waals heterostructure with high solar power conversion efficiency. Applied Surface Science, 2022, 591, 153232.	6.1	8
121	Ab initio study of spectroscopic constants and anharmonic force field of FCO2 radical. Computational and Theoretical Chemistry, 2010, 951, 77-81.	1.5	7
122	Theoretical study on the complexes of He, Ne and Ar. Chinese Physics B, 2010, 19, 123102.	1.4	7
123	The analytical potential energy functions, spectroscopic parameters and ro-vibrational spectra of SH+ molecule. Computational and Theoretical Chemistry, 2012, 979, 44-48.	2.5	7
124	The effects of collision energy and reagent vibrational excitation on the reactivity of the reaction H+LiH: A quasiclassical trajectory study. Computational and Theoretical Chemistry, 2013, 1006, 31-36.	2.5	7
125	Influence of collision energy and reagent vibrational excitation on the stereodynamics of the reaction H + LiH â†' H2+ Li. Chemical Physics, 2013, 415, 8-13.	1.9	7
126	First-principles analysis of the effect of contact sites on electronic transport properties of diaminofluorene. Physica B: Condensed Matter, 2013, 417, 70-74.	2.7	7

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127	Electronic structure of Zn doped Ga0.5Al0.5As photocathodes from first-principles. Solid State Communications, 2013, 164, 50-53.	1.9	7
128	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.	6.1	7
129	Ab Initio Studies on Spectroscopic Constants for the HAsO Molecule. Journal of Physical Chemistry A, 2017, 121, 7009-7015.	2.5	7
130	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.	3.9	7
131	High mobility and photocatalytic properties of NaXO2(X=Co, Rh, Ir). Vacuum, 2019, 168, 108824.	3.5	7
132	Newfound two-dimensional Bi2Se3 monolayers for driving hydrogen evolution reaction with the visible-light. Applied Surface Science, 2021, 564, 150389.	6.1	7
133	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.	3.9	7
134	A density functional theory study on the role of His-107 in arylamine N-acetyltransferase 2 acetylation. Biophysical Chemistry, 2006, 122, 215-220.	2.8	6
135	The molecular structure and vibrational spectra of corrolazine metal complexes (CzM) by density functional theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 64, 795-800.	3.9	6
136	Structural, electronic, and magnetic properties of (n+m=5) clusters. Computational and Theoretical Chemistry, 2010, 957, 26-30.	1.5	6
137	Ab initioinvestigations of the charge transport properties of endohedralM@C₂₀(M= Na and K) metallofullerenes. Chinese Physics B, 2010, 19, 113402.	1.4	6
138	Spectroscopic properties and vibrational levels for X2Î£+ and A2Î states of CS+ molecule: A multi-reference configuration interaction study. Computational and Theoretical Chemistry, 2011, 976, 94-97.	2.5	6
139	Comparative study of adsorption characteristics of Cs on the GaN (0001) and GaN (000Ì„) surfaces. Chinese Physics B, 2012, 21, 067103.	1.4	6
140	DENSITY FUNCTIONAL THEORY STUDIES OF SPECTROSCOPIC CONSTANTS AND ANHARMONIC FORCE FIELD OF O³⁵ClO. Journal of Theoretical and Computational Chemistry, 2013, 12, 1250117.	1.8	6
141	Influence of Vacancy Defect on Surface Feature and Adsorption of Cs on GaN(0001) Surface. Scientific World Journal, The, 2014, 2014, 1-6.	2.1	6
142	First-principles studies of electronic structure and optical properties of GaN surface doped with Si. Optik, 2014, 125, 2234-2238.	2.9	6
143	Cesium, oxygen coadsorption on AlGaN(0001) surface: experimental research and ab initio calculations. Journal of Materials Science: Materials in Electronics, 2015, 26, 2181-2188.	2.2	6
144	Cesium adsorption on In0.53Ga0.47As (100) Î²2 (2Ã—4) surface: A first-principles research. Applied Surface Science, 2015, 324, 547-553.	6.1	6

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145	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.	3.9	6
146	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.	2.5	6
147	Effects of transport direction and carrier concentration on the thermoelectric properties of AgIn5Te8: A first-principles study. Materials Research Bulletin, 2019, 113, 77-83.	5.2	6
148	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.	3.9	6
149	Numerical simulation of temperature field in crack of supercritical carbon dioxide fracturing. Energy Science and Engineering, 2020, 8, 2141-2150.	4.0	6
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