Jyh-Chiang Jiang

List of Publications by Citations

151 papers	3,444 citations	30 h-index	49 g-index
156 ext. papers	3,735 ext. citations	4.7 avg, IF	5.34 L-index

#	Paper	IF	Citations
151	Infrared Spectra of H+(H2O)5-8 Clusters: Evidence for Symmetric Proton Hydration. *Journal of the American Chemical Society*, **2000**, 122, 1398-1410	16.4	309
150	Protonated clathrate cages enclosing neutral water molecules: (H+)(H2O)21 and (H+)(H2O)28. *Journal of Chemical Physics*, **2005**, 122, 074315	3.9	139
149	Molecular Design of Porphyrins for Dye-Sensitized Solar Cells: A DFT/TDDFT Study. *Journal of Physical Chemistry Letters*, **2013**, 4, 524-30	6.4	104
148	Structures and Isomeric Transitions of NH4+(H2O)3-6: From Single to Double Rings. *Journal of the American Chemical Society*, **1998**, 120, 8777-8788	16.4	104
147	Efficient hydrogen storage in boron doped graphene decorated by transition metals □A first-principles study. *Carbon*, **2014**, 73, 132-140	10.4	99
146	Hydrogen bond stabilization in 1,3-dimethylimidazolium methyl sulfate and 1-butyl-3-methylimidazolium hexafluorophosphate probed by high pressure: the role of charge-enhanced C-H...O interactions in the room-temperature ionic liquid. *Journal of Physical Chemistry B*, **2006**, 110, 3302-7	3.4	96
145	Structural organization in aqueous solutions of 1-Butyl-3-methylimidazolium halides: a high-pressure infrared spectroscopic study on ionic liquids. *Journal of Physical Chemistry B*, **2008**, 112, 4351-6	3.4	78
144	C□H□ Bond Activation of Methane via □ Interaction on the IrO2(110) Surface: Density Functional Theory Study. *Journal of Physical Chemistry C*, **2012**, 116, 6367-6370	3.8	75
143	Cooperative effect of unsheltered amide groups on CO2 adsorption inside open-ended channels of a zinc(II)-organic framework. *Inorganic Chemistry*, **2013**, 52, 3962-8	5.1	71
142	Theoretical study on the correlation between band gap, bandwidth, and oscillator strength in fluorene-based donor-acceptor conjugated copolymers. *Journal of Physical Chemistry B*, **2009**, 113, 8268-77	3.4	64
141	Evidence of rotational isomerism in 1-butyl-3-methylimidazolium halides: a combined high-pressure infrared and Raman spectroscopic study. *Journal of Physical Chemistry A*, **2007**, 111, 9201-6	2.8	60
140	C[bond]H- - -O hydrogen bonds in beta-sheetlike networks: combined X-ray crystallography and high-pressure infrared study. *Journal of the American Chemical Society*, **2003**, 125, 12358-64	16.4	57
139	Isomeric Transitions between Linear and Cyclic H+(CH3OH)4,5:□Implications for Proton Migration in Liquid Methanol. *Journal of Physical Chemistry A*, **1999**, 103, 2941-2944	2.8	56
138	Theoretical study of the reductive decomposition of ethylene sulfite: a film-forming electrolyte additive in lithium ion batteries. *Journal of Physical Chemistry A*, **2012**, 116, 11025-33	2.8	51
137	Migration of an Excess Proton upon Asymmetric Hydration: H+[(CH3)2O](H2O)n as a Model System. *Journal of the American Chemical Society*, **1999**, 121, 4443-4450	16.4	48
136	Effects of water and methanol on the molecular organization of 1-butyl-3-methylimidazolium tetrafluoroborate as functions of pressure and concentration. *Journal of Chemical Physics*, **2008**, 129, 044506	3.9	45
135	Theoretical study of the reductive decomposition of 1,3-propane sultone: SEI forming additive in lithium-ion batteries. *RSC Advances*, **2012**, 2, 5439	3.7	42

134	Lithium diffusion in graphene and graphite: Effect of edge morphology. *Carbon*, **2016**, 103, 209-216	10.4	40
133	Photoisomerization and photodissociation of toluene in molecular beam. *Journal of the American Chemical Society*, **2002**, 124, 4068-75	16.4	39
132	Comparative Study on the Solid Electrolyte Interface Formation by the Reduction of Alkyl Carbonates in Lithium ion Battery. *Electrochimica Acta*, **2014**, 136, 274-285	6.7	38
131	Structural change of ionic association in ionic liquid/water mixtures: a high-pressure infrared spectroscopic study. *Journal of Chemical Physics*, **2009**, 130, 124503	3.9	38
130	Novel triarylamine-based alternating conjugated polymer with high hole mobility: Synthesis, electro-optical, and electronic properties. *Journal of Polymer Science Part A*, **2010**, 48, 4654-4667	2.5	38
129	High-pressure spectroscopic probe of hydrophobic hydration of the methyl groups in dimethyl sulfoxide. *Journal of Chemical Physics*, **2003**, 118, 1802-1807	3.9	37
128	First principles study of organic sensitizers for dye sensitized solar cells: effects of anchoring groups on optoelectronic properties and dye aggregation. *Physical Chemistry Chemical Physics*, **2016**, 18, 1071-81	3.6	36
127	Design strategies of metal free-organic sensitizers for dye sensitized solar cells: Role of donor and acceptor monomers. *Organic Electronics*, **2014**, 15, 1205-1214	3.5	36
126	Novel rapid switching and bleaching electrochromic polyimides containing triarylamine with 2-phenyl-2-isopropyl groups. *Polymer*, **2010**, 51, 4493-4502	3.9	33
125	A First Principles study on Boron-doped Graphene decorated by Ni-Ti-Mg atoms for Enhanced Hydrogen Storage Performance. *Scientific Reports*, **2015**, 5, 16797	4.9	32
124	Preparation and oxygen reduction activity of stable RuSex/C catalyst with pyrite structure. *Electrochimica Acta*, **2009**, 54, 4297-4304	6.7	31
123	Photodissociation of ethylbenzene and n-propylbenzene in a molecular beam. *Journal of Chemical Physics*, **2002**, 117, 7034-7040	3.9	31
122	Conformations of 1-Butyl-3-methylimidazolium Chloride Probed by High Pressure Raman Spectroscopy. *International Journal of Molecular Sciences*, **2006**, 7, 417-424	6.3	30
121	Evidence of charge-enhanced CHO interactions in aqueous protonated imidazole probed by high pressure infrared spectroscopy. *Journal of Chemical Physics*, **2003**, 119, 10753-10758	3.9	30
120	Evidence for hydrogen bond-like CHO interactions in aqueous 1,4-dioxane probed by high pressure. *Chemical Physics Letters*, **2004**, 397, 205-210	2.5	29
119	Effect of External Electric Field on Methane Conversion on IrO2(110) Surface: A Density Functional Theory Study. *ACS Catalysis*, **2019**, 9, 8230-8242	13.1	27
118	Solvation and microscopic properties of ionic liquid/acetonitrile mixtures probed by high-pressure infrared spectroscopy. *Journal of Chemical Physics*, **2009**, 131, 234502	3.9	27
117	Interactions of Silica Nanoparticles and Ionic Liquids Probed by High Pressure Vibrational Spectroscopy. *Journal of Physical Chemistry C*, **2011**, 115, 11962-11967	3.8	26

116	Ab initio study of the ammoniated ammonium ions NH4+(NH3)0–8. *Chemical Physics*, **2002**, 276, 93-106	2.3	26
115	Evidence for C–H···O interaction of acetone and deuterium oxide probed by high-pressure. *Journal of Chemical Physics*, **2001**, 115, 3215-3218	3.9	26
114	Aqueous solution-processed off-stoichiometric CuInS QDs and their application in quantum dot-sensitized solar cells. *Journal of Materials Chemistry A*, **2018**, 6, 9629-9641	13	25
113	Association structures of ionic liquid–DMSO mixtures studied by high-pressure infrared spectroscopy. *Journal of Chemical Physics*, **2011**, 134, 044506	3.9	25
112	Photoionization of methanol dimer using a tunable vacuum ultraviolet laser. *Journal of Chemical Physics*, **1999**, 111, 3434-3440	3.9	25
111	Hydrogen-Bond Rearrangement and Intermolecular Proton Transfer in Protonated Methanol Clusters. *Israel Journal of Chemistry*, **1999**, 39, 231-243	3.4	25
110	A High-Pressure Study of the Effects of TiO2 Nanoparticles on the Structural Organization of Ionic Liquids. *Journal of Physical Chemistry C*, **2011**, 115, 23778-23783	3.8	24
109	The intramolecular blue-shifting C–H···F–C hydrogen bond: crystal structure of [4,4?-bis(HCF2CF2CF2CF2CH2OCH2)-2,2?-bpy]MCl2 where M = Pt, Pd. *CrystEngComm*, **2010**, 12, 538-542	3.3	24
108	Carbon-carbon bond cleavage in the photoionization of ethanol and 1-propanol clusters. *Journal of Chemical Physics*, **2004**, 120, 8979-84	3.9	24
107	Photodissociation dynamics of fluorobenzene. *Journal of the American Chemical Society*, **2003**, 125, 9814-20	13.4	24
106	Probing C-H...X hydrogen bonds in amide-functionalized imidazolium salts under high pressure. *Journal of Chemical Physics*, **2004**, 120, 8645-50	3.9	24
105	Photodissociation of ethylbenzene at 248 nm. *Journal of Chemical Physics*, **2002**, 116, 7779-7782	3.9	24
104	Charge-enhanced C–H···O interactions of a self-assembled triple helical spine probed by high-pressure. *Journal of Chemical Physics*, **2002**, 117, 1723-1728	3.9	24
103	Transmissive-to-black fast electrochromic switching from a long conjugated pendant group and a highly dispersed polymer/SWNT. *Polymer Chemistry*, **2018**, 9, 619-626	4.9	23
102	Revealing the influence of Cyano in Anchoring Groups of Organic Dyes on Adsorption Stability and Photovoltaic Properties for Dye-Sensitized Solar Cells. *Scientific Reports*, **2017**, 7, 4979	4.9	23
101	Oxidative decomposition of propylene carbonate in lithium ion batteries: a DFT study. *Journal of Physical Chemistry A*, **2013**, 117, 7959-69	2.8	22
100	Probing the Nature and Local Structure of Phosphonic Acid Groups Functionalized in Mesoporous Silica SBA-15. *Journal of Physical Chemistry C*, **2012**, 116, 1658-1669	3.8	22
99	Adsorption and Thermal Reactions of H2O and H2S on Ge(100). *Journal of Physical Chemistry C*, **2010**, 114, 1019-1027	3.8	22

98	Density Functional Theory Study of the Oxidation of Ammonia on RuO2(110) Surface. *Journal of Physical Chemistry C*, **2009**, 113, 17411-17417	3.8	22
97	DFT Study of NHx (x = 1□) Adsorption on RuO2(110) Surfaces. *Journal of Physical Chemistry C*, **2009**, 113, 2816-2821	3.8	22
96	Hydrogen bond-like equatorial C□H?O interactions in aqueous 1,3-dioxane: A combined high-pressure infrared and Raman spectroscopy study. *Chemical Physics Letters*, **2005**, 410, 42-48	2.5	22
95	Novel poly(triphenylamine-alt-fluorene) with asymmetric hexaphenylbenzene and pyrene moieties: synthesis, fluorescence, flexible near-infrared electrochromic devices and theoretical investigation. *Polymer Chemistry*, **2016**, 7, 1505-1516	4.9	21
94	Boron and Nitrogen Co-doped Graphene Used As Counter Electrode for Iodine Reduction in Dye-Sensitized Solar Cells. *Journal of Physical Chemistry C*, **2018**, 122, 26385-26392	3.8	21
93	Barrierless proton transfer within short protonated peptides in the presence of water bridges. A density functional theory study. *Journal of Physical Chemistry B*, **2011**, 115, 1485-90	3.4	20
92	Deoxygenation of IrO2(110) surface: Core-level spectroscopy and density functional theory calculation. *Surface Science*, **2010**, 604, 118-124	1.8	20
91	Experimental and theoretical investigation of a new rapid switching near-infrared electrochromic conjugated polymer. *Journal of Polymer Science Part A*, **2010**, 48, 3913-3923	2.5	20
90	Correlation of Mesh Size of Metal□arboxylate Layer with Degree of Interpenetration in Pillared-Layer Frameworks. *Crystal Growth and Design*, **2014**, 14, 5608-5616	3.5	19
89	Theoretical investigations of metal-free dyes for solar cells: Effects of electron donor and acceptor groups on sensitizers. *Journal of Power Sources*, **2013**, 242, 464-471	8.9	18
88	Density Functional Theory Study of NHx (x = 0□) and N2 Adsorption on IrO2(110) Surfaces. *Journal of Physical Chemistry C*, **2010**, 114, 18588-18593	3.8	18
87	A DFT study of ethanol adsorption and decomposition on □Al2O3(0001) surface. *Applied Surface Science*, **2016**, 363, 636-643	6.7	17
86	Density functional theory study of the oxidation of ammonia on the IrO2(110) surface. *Langmuir*, **2011**, 27, 14253-9	4	17
85	A DFT study of ethane activation on IrO 2 (110) surface by precursor-mediated mechanism. *Applied Catalysis A: General*, **2017**, 541, 8-14	5.1	16
84	A combined experimental and theoretical study of surface film formation: Effect of oxygen on the reduction mechanism of propylene carbonate. *Journal of Power Sources*, **2013**, 244, 318-327	8.9	16
83	On the search for C□H□O hydrogen bonding in aqueous acetic acid: Combined high-pressure infrared spectroscopy and ab initio calculations study. *Journal of Chemical Physics*, **2002**, 117, 3799-3803	3.9	16
82	Microkinetic Simulation of Ammonia Oxidation on the RuO2(110) Surface. *ACS Catalysis*, **2014**, 4, 639-648	13.1	15
81	Conjugated polymers containing electron-deficient main chains and electron-rich pendant groups: Synthesis and application to electroluminescence. *Organic Electronics*, **2011**, 12, 1048-1062	3.5	15

80	Local structures of water in 1-butyl-3-methylimidazolium tetrafluoroborate probed by high-pressure infrared spectroscopy. *Analytical Sciences*, **2008**, 24, 1305-9	1.7	15
79	High-pressure Raman studies on aqueous protonated thiazole: presence of charge-enhanced C-H...O hydrogen bonds. *Journal of Physical Chemistry B*, **2005**, 109, 23103-7	3.4	15
78	Pressure-Enhanced CHIIIO Interactions in Aqueous tert-Butyl Alcohol. *Journal of Physical Chemistry A*, **2004**, 108, 11001-11005	2.8	15
77	In situ spectroscopic and theoretical investigation of methane activation on IrO2 nanoparticles: Role of Ir oxidation state on C-H activation. *Journal of Catalysis*, **2020**, 385, 265-273	7.3	15
76	Enhanced moisture stability of cesium lead iodide perovskite solar cells - a first-principles molecular dynamics study. *Physical Chemistry Chemical Physics*, **2020**, 22, 5693-5701	3.6	14
75	Photoisomerization and Photodissociation of m-Xylene in a Molecular Beam. *Journal of Physical Chemistry A*, **2003**, 107, 4019-4024	2.8	14
74	Amide-containing zinc(II) metal□organic layered networks: a structure□CO2 capture relationship. *Inorganic Chemistry Frontiers*, **2015**, 2, 477-484	6.8	13
73	Methanol decomposition reactions over a boron-doped graphene supported Ru-Pt catalyst. *Physical Chemistry Chemical Physics*, **2018**, 20, 9355-9363	3.6	13
72	Microkinetic Simulation of Temperature-Programmed Desorption. *Journal of Physical Chemistry C*, **2013**, 117, 6136-6142	3.8	13
71	Neutrally colourless, transparent and thermally stable polynorbornenes via ring-opening metathesis polymerisation for near-infrared electroactive applications. *Journal of Materials Chemistry*, **2011**, 21, 8597		13
70	A high-pressure infrared spectroscopic study on the interaction of ionic liquids with PEO-PPO-PEO block copolymers and 1,4-dioxane. *Journal of Physical Chemistry B*, **2011**, 115, 883-8	3.4	13
69	Synthesis and computational oxidation mechanism study of novel organosoluble aramids with high modulus by low-temperature solution polycondensation. *Journal of Polymer Science Part A*, **2010**, 48, 5659-5669	2.5	13
68	On the Search for H5O2+centered Water Clusters in the Gas Phase. *Journal of the Chinese Chemical Society*, **1999**, 46, 427-434	1.5	13
67	Dopamine sensing by boron and nitrogen co-doped single-walled carbon nanotubes: A first-principles study. *Applied Surface Science*, **2019**, 473, 59-64	6.7	13
66	Theoretical study on molecular design and optical properties of organic sensitizers. *Physical Chemistry Chemical Physics*, **2014**, 16, 15389-99	3.6	12
65	Proton-Assisted Hydration at Hydrophobic Sites in Protonated Ether and Keto Dimers. *Journal of Physical Chemistry A*, **1999**, 103, 8753-8761	2.8	12
64	Amide-CO2 Interaction Induced Gate-Opening Behavior for CO2 Adsorption in 2-Fold Interpenetrating Framework. *ChemistrySelect*, **2016**, 1, 2923-2929	1.8	11
63	High-Purity Semiconducting Single-Walled Carbon Nanotubes via Selective Dispersion in Solution Using Fully Conjugated Polytriarylamines. *Macromolecules*, **2016**, 49, 8520-8529	5.5	11

62	Density functional theory study of ethanol decomposition on 3Ni/□Al□(0001) surface. *Langmuir*, **2010**, 26, 15845-51	4	11
61	The role of charge-enhanced C□H?O interactions in gel-like mixtures prepared from ionic liquids and tungsten(VI) oxide nanoparticles. *Chemical Physics Letters*, **2006**, 427, 310-316	2.5	11
60	Comparative Studies of H+(C6H6)(H2O)1,2 and H+(C5H5N)(H2O)1,2 by DFT Calculations and IR Spectroscopy. *Australian Journal of Chemistry*, **2004**, 57, 1153	1.2	11
59	New Insights into the N-S Bond Formation of a Sulfurized-Polyacrylonitrile Cathode Material for Lithium-Sulfur Batteries. *ACS Applied Materials & Interfaces*, **2021**, 13, 14230-14238	9.5	11
58	Understanding the Role of Dopant Metal Atoms on the Structural and Electronic Properties of Lithium-Rich LiNiMnO Cathode Material for Lithium-Ion Batteries. *Journal of Physical Chemistry Letters*, **2019**, 10, 4842-4850	6.4	10
57	Surface Raman Spectroscopy of trans-Stilbene on Ag/Ge(111): Surface-Induced Effects. *Journal of Physical Chemistry C*, **2009**, 113, 208-212	3.8	10
56	Characterization of extraframework aluminum in H-mordenite dealuminated with ammonium hexafluorosilicate. *Catalysis Today*, **2004**, 97, 13-23	5.3	10
55	Initial growth of chemical-vapor-deposited Ru from bis(hexafluoroacetylacetonate)dicarbonyl ruthenium. *Thin Solid Films*, **2005**, 483, 31-37	2.2	10
54	Effects of the terminal donor unit in dyes with D-D-□A architecture on the regeneration mechanism in DSSCs: a computational study. *Physical Chemistry Chemical Physics*, **2018**, 20, 23564-23577	3.6	10
53	A first principles study of CO oxidation over gold clusters: The catalytic role of boron nitride support and water. *Molecular Catalysis*, **2019**, 471, 44-53	3.3	9
52	Pressure-enhanced surface interactions between nano-TiO□and ionic liquid mixtures probed by high pressure IR spectroscopy. *Physical Chemistry Chemical Physics*, **2015**, 17, 21143-8	3.6	9
51	Adsorption and Decomposition of Ethylene Carbonate on LiMn2O4 Cathode Surface. *Electrochimica Acta*, **2016**, 210, 61-70	6.7	9
50	Density Functional Theory Study of Water-Gas-Shift Reaction on 3Cu/□Al2O3(0001) Surface. *Journal of Physical Chemistry C*, **2013**, 117, 12045-12053	3.8	9
49	Preparation of neutrally colorless, transparent polynorbornenes with multiple redox-active chromophores via ring-opening metathesis polymerization toward electrochromic applications. *Journal of Polymer Science Part A*, **2011**, 49, 3248-3259	2.5	9
48	Mechanism of growth of the Ge wetting layer upon exposure of Si(100)-2 x 1 to GeH4. *Journal of the American Chemical Society*, **2008**, 130, 5440-2	16.4	9
47	Temperature-programmed desorption studies of NH and HO on the RuO(110) surface: effects of adsorbate diffusion. *Physical Chemistry Chemical Physics*, **2018**, 20, 24201-24209	3.6	9
46	New Insights into Organic Dye Regeneration Mechanism in Dye-Sensitized Solar Cells: A Theoretical Study. *ACS Sustainable Chemistry and Engineering*, **2017**, 5, 8619-8629	8.3	8
45	Application of Density Functional Theory and Photoelectron Spectra to the Adsorption and Reaction of H2S on Si (100). *Journal of Physical Chemistry C*, **2011**, 115, 19203-19209	3.8	8

44	Energetics and Rate Constants of Si2H6 and Ge2H6 Dissociative Adsorption on Dimers of SiGe(100)-2 □1. *Journal of Physical Chemistry C*, **2007**, 111, 13466-13472	3.8	8
43	The effect of pressure on charge-enhanced C□H?O interactions in aqueous triethylamine hydrochloride probed by high pressure Raman spectroscopy. *Chemical Physics Letters*, **2006**, 432, 100-105	2.5	8
42	DFT study on dissociative adsorption of SiH4 and GeH4 on SiGe(100)-2□1 surface. *Surface Science*, **2006**, 600, 3194-3201	1.8	8
41	Pressure-dependent studies on hydration of the C□H group in formic acid. *Journal of Chemical Physics*, **2001**, 115, 8032-8037	3.9	8
40	Reduction mechanism of iron titanium based oxygen carriers with H2 for chemical looping applications □a combined experimental and theoretical study. *RSC Advances*, **2016**, 6, 106340-106346	3.7	8
39	Effect of solvent proton affinity on the kinetics of michael addition polymerization of n,n?-bismaleimide-4,4?-diphenylmethane with barbituric acid. *Polymer Engineering and Science*, **2014**, 54, 559-568	2.3	7
38	Theoretical Study of Electrochemical and Electrochromic Properties of Novel Viologen Derivatives: Effects of Donors and □Conjugation. *Journal of Physical Chemistry B*, **2019**, 123, 4735-4744	3.4	6
37	A first principles study of H2S adsorption and decomposition on a Ge(100) surface. *RSC Advances*, **2015**, 5, 3825-3832	3.7	6
36	Enhancement of chlorobenzene sensing by doping aluminum on nanotubes: A DFT study. *Applied Surface Science*, **2020**, 514, 145897	6.7	6
35	Quantum Chemical Studies of Methane Oxidation to Methanol on a Biomimetic Tricopper Complex: Mechanistic Insights. *ChemistrySelect*, **2018**, 3, 5113-5122	1.8	6
34	Specific interactions between the quaternary ammonium oligoether-based ionic liquid and water as a function of pressure. *Physical Chemistry Chemical Physics*, **2013**, 15, 12734-41	3.6	6
33	Intermolecular Interactions in Aqueous Dimethyl Sulphoxide and Acetic Acid Probed by High-Pressure FTIR. *Journal of the Chinese Chemical Society*, **2002**, 49, 663-667	1.5	5
32	Theoretical study on halide and mixed halide Perovskite solar cells: Effects of halide atoms on the stability and electronic properties. *Journal of the Chinese Chemical Society*, **2019**, 66, 575-582	1.5	5
31	A theoretical design of some silole-based dibenzothiophene-S,S-dioxide semiconducting compounds for red phosphorescence. *Organic Electronics*, **2018**, 54, 270-276	3.5	4
30	Theoretical Study of the Reductive Decomposition of Vinylethylene Sulfite as an Additive in Lithium Ion Battery. *Journal of the Chinese Chemical Society*, **2016**, 63, 480-487	1.5	4
29	Theoretical studies on effective metal-to-ligand charge transfer characteristics of novel ruthenium dyes for dye sensitized solar cells. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 565-75	4.2	4
28	Spin-polarized transport properties in some transition metal dithiolene complexes. *Physical Chemistry Chemical Physics*, **2017**, 19, 32536-32543	3.6	4
27	Unraveling Molecular Adsorption with Surface Raman Spectroscopy: trans-Stilbene, trans,trans-Distyrylbenzene, and trans-Azobenzene on Ag/Ge(111). *Journal of Physical Chemistry C*, **2011**, 115, 516-520	3.8	4

26	Study of Pathway of Hydrogen Migration and Desorption on SiGe(100) Surface UsingAb InitioCalculations. *Japanese Journal of Applied Physics*, **2005**, 44, 7625-7633	1.4	4
25	Comparable catalytic activity of a low-cost catalyst IrO2/TiO2 for methane conversion A density functional theory study. *Applied Surface Science*, **2021**, 151938	6.7	4
24	Theoretical study on the interaction of iodide electrolyte/organic dye with the TiO surface in dye-sensitized solar cells. *Physical Chemistry Chemical Physics*, **2020**, 22, 26410-26418	3.6	4
23	Effects of Electric Field on the Performance of Graphene-Based Counter Electrodes for Dye-Sensitized Solar Cells: A Theoretical Study. *Journal of Physical Chemistry C*, **2019**, 123, 30373-30381	3.8	4
22	A computational study of CO oxidation on IrO2 (1 1 0) surface. *Applied Surface Science*, **2021**, 539, 148246	6.7	4
21	Tuning Interfacial Thermal and Electrical Conductance across a Metal/MoS2 Monolayer through N-Methyl-2-pyrrolidone Wet Cleaning. *Advanced Materials Interfaces*, **2020**, 7, 2000364	4.6	3
20	Silole and selenophene-based D-A dyes in dye-sensitized solar cells: Insights from optoelectronic and regeneration properties. *Dyes and Pigments*, **2020**, 176, 108243	4.6	3
19	Theoretical study on wetting behavior of B-SWNT: Effects of doping concentration. *Applied Surface Science*, **2019**, 497, 143798	6.7	3
18	Effects of hydrogen on GaN metalorganic vapor-phase epitaxy using tertiarybutylhydrazine as nitrogen source. *Journal of Crystal Growth*, **2004**, 266, 347-353	1.6	3
17	B, N-co-doped graphene-supported Ir and Pt clusters for methane activation and C-C coupling: A density functional theory study. *Journal of Computational Chemistry*, **2020**, 41, 194-202	3.5	3
16	A First Study of the Kinetics of Metal Ion Adsorption at Solid/Liquid Interface Using Evanescent Wave-Based Optical Microfiber. *IEEE Sensors Journal*, **2020**, 1-1	4	2
15	Photodissociation and photoisomerization of alpha-fluorotoluene and 4-fluorotoluene in a molecular beam. *Journal of Chemical Physics*, **2006**, 125, 133305	3.9	2
14	Hydrophobic hydration in aqueous acetic acid and formic acid solutions probed by high pressure. *Journal of Luminescence*, **2002**, 98, 177-182	3.8	2
13	Theoretical insight into hydroxyl production HO decomposition over the FeO(311) surface.. *RSC Advances*, **2021**, 11, 36257-36264	3.7	2
12	Elucidating the Improved Electrolyte Stability with Novel Benzimidazole Salt on the Li Anode Surface: Insights into Interfacial Reactions. *Journal of Physical Chemistry C*, **2020**, 124, 23523-23531	3.8	2
11	Combined Density Functional Theory and Microkinetics Study to Predict Optimum Operating Conditions of Si(100) Surface Carbonization by Acetylene for High Power Devices. *Journal of Physical Chemistry Letters*, **2021**, 12, 4558-4568	6.4	2
10	A first-principles study on double-sided decorated boron nitrogen co-doped graphene by vanadium for enhanced low-temperature reversible hydrogen storage. *Sustainable Energy and Fuels* , **2021**, 5, 2159-2168	5.8	2
9	Theoretical investigation of CO2 conversion on corrugated g-C3N4 Surface decorated by single-atom of Fe, Co, and Pd. *Molecular Catalysis*, **2022**, 526, 112402	3.3	2

8	An Experimental Study on the Reduction Kinetics of Iron Titanium Based Oxygen Carriers with CO Validated by First Principle Calculations. *ChemistrySelect*, **2017**, 2, 274-278	1.8	1
7	Quantum chemical study on the gas-phase reaction of tertiarybutylhydrazine: A potential nitrogen-bearing compound for GaN film growth. *Thin Solid Films*, **2006**, 498, 100-107	2.2	1
6	Intermolecular Hydrogen Bonding and Structures in 1,3-Dioxane/D2O Mixtures Studied by High-Pressure Raman Spectroscopy. *Journal of the Chinese Chemical Society*, **2005**, 52, 625-630	1.5	1
5	The fluorescence turn-off mechanism of a norbornene-derived homopolymer an Al3+ colorimetric and fluorescent chemosensor. *Materials Advances*,	3.3	1
4	Direct visualization of lattice oxygen evolution and related electronic properties of Li1.2Ni0.2Mn0.6O2 cathode materials. *Applied Surface Science*, **2021**, 563, 150334	6.7	1
3	The investigation of methane storage at the Ni-MOF-74 material: a periodic DFT calculation. *Physical Chemistry Chemical Physics*, **2021**, 23, 12270-12279	3.6	1
2	Boron and Nitrogen Codoped Multilayer Graphene as a Counter Electrode: A Combined Theoretical and Experimental Study on Dye-Sensitized Solar Cells under Ambient Light Conditions. *Journal of Physical Chemistry C*, **2021**, 125, 24894-24901	3.8	1
1	The role of donors/acceptors in molecular rotors towards development of ambient blue light sensors - A density functional theory study. *Materials Chemistry and Physics*, **2022**, 277, 125563	4.4	