Jyh-Chiang Jiang

List of Publications by Year
in descending order

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154	4,063	136740	161609
papers	citations	32 h-index	54 g-index

156	156	156	4408
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Infrared Spectra of H+(H2O)5-8Clusters:Â Evidence for Symmetric Proton Hydration. Journal of the American Chemical Society, 2000, 122, 1398-1410.	6.6	337
2	Protonated clathrate cages enclosing neutral water molecules: H+(H2O)21 and H+(H2O)28. Journal of Chemical Physics, 2005, 122, 074315.	1.2	144
3	Molecular Design of Porphyrins for Dye-Sensitized Solar Cells: A DFT/TDDFT Study. Journal of Physical Chemistry Letters, 2013, 4, 524-530.	2.1	123
4	Efficient hydrogen storage in boron doped graphene decorated by transition metals â€“ A first-principles study. Carbon, 2014, 73, 132-140.	5.4	123
5	Structures and Isomeric Transitions of NH4+(H2O)3-6:â€‰ From Single to Double Rings. Journal of the American Chemical Society, 1998, 120, 8777-8788.	6.6	113
6	Hydrogen Bond Stabilization in 1,3-Dimethylimidazolium Methyl Sulfate and 1-Butyl-3-Methylimidazolium Hexafluorophosphate Probed by High Pressure:â€‰ The Role of Charge-Enhanced Câ^'HÂ·Â·Â·O Interactions in the Room-Temperature Ionic Liquid. Journal of Physical Chemistry B, 2006, 110, 3302-3307.	1.2	99
7	Câ€“H Bond Activation of Methane via Ïƒâ€“d Interaction on the IrO₂(110) Surface: Density Functional Theory Study. Journal of Physical Chemistry C, 2012, 116, 6367-6370.	1.5	95
8	Cooperative Effect of Unsheltered Amide Groups on CO₂ Adsorption Inside Open-Ended Channels of a Zinc(II)â€“Organic Framework. Inorganic Chemistry, 2013, 52, 3962-3968.	1.9	82
9	Structural Organization in Aqueous Solutions of 1-Butyl-3-methylimidazolium Halides:Â A High-Pressure Infrared Spectroscopic Study on Ionic Liquids. Journal of Physical Chemistry B, 2008, 112, 4351-4356.	1.2	80
10	Theoretical Study on the Correlation between Band Gap, Bandwidth, and Oscillator Strength in Fluorene-Based Donorâ^'Acceptor Conjugated Copolymers. Journal of Physical Chemistry B, 2009, 113, 8268-8277.	1.2	70
11	Câ^'H-Â-Â-O Hydrogen Bonds in Î²-Sheetlike Networks:Â Combined X-ray Crystallography and High-Pressure Infrared Study. Journal of the American Chemical Society, 2003, 125, 12358-12364.	6.6	62
12	Evidence of Rotational Isomerism in 1-Butyl-3-methylimidazolium Halides:Â A Combined High-Pressure Infrared and Raman Spectroscopic Studyâ€. Journal of Physical Chemistry A, 2007, 111, 9201-9206.	1.1	62
13	Isomeric Transitions between Linear and Cyclic H+(CH3OH)4,5:Â Implications for Proton Migration in Liquid Methanol. Journal of Physical Chemistry A, 1999, 103, 2941-2944.	1.1	61
14	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, 11025-11033.	1.1	58
15	Lithium diffusion in graphene and graphite: Effect of edge morphology. Carbon, 2016, 103, 209-216.	5.4	53
16	Migration of an Excess Proton upon Asymmetric Hydration:â€‰ H+[(CH3)2O](H2O)n as a Model System. Journal of the American Chemical Society, 1999, 121, 4443-4450.	6.6	49
17	A First Principles study on Boron-doped Graphene decorated by Ni-Ti-Mg atoms for Enhanced Hydrogen Storage Performance. Scientific Reports, 2015, 5, 16797.	1.6	49
18	Theoretical study of the reductive decomposition of 1,3-propane sultone: SEI forming additive in lithium-ion batteries. RSC Advances, 2012, 2, 5439.	1.7	48

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19	Comparative Study on the Solid Electrolyte Interface Formation by the Reduction of Alkyl Carbonates in Lithium ion Battery. Electrochimica Acta, 2014, 136, 274-285.	2.6	48
20	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.	1.2	46
21	Structural change of ionic association in ionic liquid/water mixtures: A high-pressure infrared spectroscopic study. Journal of Chemical Physics, 2009, 130, 124503.	1.2	43
22	Photoisomerization and Photodissociation of Toluene in Molecular Beam. Journal of the American Chemical Society, 2002, 124, 4068-4075.	6.6	41
23	Design strategies of metal free-organic sensitizers for dye sensitized solar cells: Role of donor and acceptor monomers. Organic Electronics, 2014, 15, 1205-1214.	1.4	41
24	High-pressure spectroscopic probe of hydrophobic hydration of the methyl groups in dimethyl sulfoxide. Journal of Chemical Physics, 2003, 118, 1802-1807.	1.2	40
25	Novel triarylamineâ€based alternating conjugated polymer with high hole mobility: Synthesis, electroâ€optical, and electronic properties. Journal of Polymer Science Part A, 2010, 48, 4654-4667.	2.5	40
26	Aqueous solution-processed off-stoichiometric Cuâ€“Inâ€“S QDs and their application in quantum dot-sensitized solar cells. Journal of Materials Chemistry A, 2018, 6, 9629-9641.	5.2	40
27	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, 1071-1081.	1.3	39
28	Conformations of 1-Butyl-3-methylimidazolium Chloride Probed by High Pressure Raman Spectroscopy. International Journal of Molecular Sciences, 2006, 7, 417-424.	1.8	36
29	Novel rapid switching and bleaching electrochromic polyimides containing triarylamine with 2-phenyl-2-isopropyl groups. Polymer, 2010, 51, 4493-4502.	1.8	35
30	Preparation and oxygen reduction activity of stable RuSex/C catalyst with pyrite structure. Electrochimica Acta, 2009, 54, 4297-4304.	2.6	34
31	Effect of External Electric Field on Methane Conversion on IrO₂(110) Surface: A Density Functional Theory Study. ACS Catalysis, 2019, 9, 8230-8242.	5.5	34
32	Photodissociation of ethylbenzene and n-propylbenzene in a molecular beam. Journal of Chemical Physics, 2002, 117, 7034-7040.	1.2	33
33	New Insights into the Nâ€“S Bond Formation of a Sulfurized-Polyacrylonitrile Cathode Material for Lithiumâ€“Sulfur Batteries. ACS Applied Materials & Interfaces, 2021, 13, 14230-14238.	4.0	33
34	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.	1.5	31
35	Evidence of charge-enhanced Câ€“Hâ€“O interactions in aqueous protonated imidazole probed by high pressure infrared spectroscopy. Journal of Chemical Physics, 2003, 119, 10753-10758.	1.2	30
36	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.	1.6	30

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37	Hydrogenâ€Bond Rearrangement and Intermolecular Proton Transfer in Protonated Methanol Clusters. Israel Journal of Chemistry, 1999, 39, 231-243.	1.0	29
38	Evidence for hydrogen bond-like Câ€“Hâ€“O interactions in aqueous 1,4-dioxane probed by high pressure. Chemical Physics Letters, 2004, 397, 205-210.	1.2	29
39	Solvation and microscopic properties of ionic liquid/acetonitrile mixtures probed by high-pressure infrared spectroscopy. Journal of Chemical Physics, 2009, 131, 234502.	1.2	29
40	Interactions of Silica Nanoparticles and Ionic Liquids Probed by High Pressure Vibrational Spectroscopy. Journal of Physical Chemistry C, 2011, 115, 11962-11967.	1.5	29
41	Association structures of ionic liquid/DMSO mixtures studied by high-pressure infrared spectroscopy. Journal of Chemical Physics, 2011, 134, 044506.	1.2	29
42	Transmissive-to-black fast electrochromic switching from a long conjugated pendant group and a highly dispersed polymer/SWNT. Polymer Chemistry, 2018, 9, 619-626.	1.9	29
43	Enhanced moisture stability of cesium lead iodide perovskite solar cells â€“ a first-principles molecular dynamics study. Physical Chemistry Chemical Physics, 2020, 22, 5693-5701.	1.3	29
44	Oxidative Decomposition of Propylene Carbonate in Lithium Ion Batteries: A DFT Study. Journal of Physical Chemistry A, 2013, 117, 7959-7969.	1.1	28
45	Dopamine sensing by boron and nitrogen co-doped single-walled carbon nanotubes: A first-principles study. Applied Surface Science, 2019, 473, 59-64.	3.1	28
46	Photoionization of methanol dimer using a tunable vacuum ultraviolet laser. Journal of Chemical Physics, 1999, 111, 3434-3440.	1.2	27
47	Charge-enhanced Câ€“Hâ€“O interactions of a self-assembled triple helical spine probed by high-pressure. Journal of Chemical Physics, 2002, 117, 1723-1728.	1.2	27
48	Photodissociation Dynamics of Fluorobenzene. Journal of the American Chemical Society, 2003, 125, 9814-9820.	6.6	27
49	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.	3.1	27
50	Evidence for Câ€“Hâ€“O interaction of acetone and deuterium oxide probed by high-pressure. Journal of Chemical Physics, 2001, 115, 3215-3218.	1.2	26
51	Ab initio study of the ammoniated ammonium ions NH4+(NH3)0â€“6. Chemical Physics, 2002, 276, 93-106.	0.9	26
52	Density Functional Theory Study of the Oxidation of Ammonia on RuO₂(110) Surface. Journal of Physical Chemistry C, 2009, 113, 17411-17417.	1.5	26
53	DFT Study of NHx (x = 1â€“3) Adsorption on RuO2(110) Surfaces. Journal of Physical Chemistry C, 2009, 113, 2816-2821.	1.5	26
54	The intramolecular blue-shifting Câ€“Hâ‹¯Fâ€“C hydrogen bond: crystal structure of [4,4â€²-bis(HCF2CF2CF2CF2CH2OCH2)-2,2â€²-bpy]MCl2where M = Pt, Pd. CrystEngComm, 2010, 12, 538-542.	1.3	26

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55	Photodissociation of ethylbenzene at 248 nm. Journal of Chemical Physics, 2002, 116, 7779-7782.	1.2	25
56	Carbonâ€“carbon bond cleavage in the photoionization of ethanol and 1-propanol clusters. Journal of Chemical Physics, 2004, 120, 8979-8984.	1.2	25
57	Probing Câ€“Hâ‹¯X hydrogen bonds in amide-functionalized imidazolium salts under high pressure. Journal of Chemical Physics, 2004, 120, 8645-8650.	1.2	25
58	Adsorption and Thermal Reactions of H₂O and H₂S on Ge(100). Journal of Physical Chemistry C, 2010, 114, 1019-1027.	1.5	25
59	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.	1.5	25
60	Methanol decomposition reactions over a boron-doped graphene supported Ruâ€“Pt catalyst. Physical Chemistry Chemical Physics, 2018, 20, 9355-9363.	1.3	25
61	Hydrogen bond-like equatorial Câ€“Hâ‹¯O interactions in aqueous 1,3-dioxane: A combined high-pressure infrared and Raman spectroscopy study. Chemical Physics Letters, 2005, 410, 42-48.	1.2	24
62	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.	1.5	24
63	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.	1.9	24
64	A DFT study of ethanol adsorption and decomposition on Î±-Al2O3(0001) surface. Applied Surface Science, 2016, 363, 636-643.	3.1	24
65	Density Functional Theory Study of NH_x (x = 0â€“3) and N₂ Adsorption on IrO₂(110) Surfaces. Journal of Physical Chemistry C, 2010, 114, 18588-18593.	1.5	23
66	Deoxygenation of IrO2(110) surface: Core-level spectroscopy and density functional theory calculation. Surface Science, 2010, 604, 118-124.	0.8	21
67	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.	4.0	21
68	Correlation of Mesh Size of Metalâ€“Carboxylate Layer with Degree of Interpenetration in Pillared-Layer Frameworks. Crystal Growth and Design, 2014, 14, 5608-5616.	1.4	21
69	Microkinetic Simulation of Ammonia Oxidation on the RuO₂(110) Surface. ACS Catalysis, 2014, 4, 639-648.	5.5	21
70	A DFT study of ethane activation on IrO 2 (110) surface by precursor-mediated mechanism. Applied Catalysis A: General, 2017, 541, 8-14.	2.2	21
71	Understanding the Role of Dopant Metal Atoms on the Structural and Electronic Properties of Lithium-Rich Li_{1.2}Ni_{0.2}Mn_{0.6}O₂ Cathode Material for Lithium-Ion Batteries. Journal of Physical Chemistry Letters, 2019, 10, 4842-4850.	2.1	21
72	Experimental and theoretical investigation of a new rapid switching nearâ€infrared electrochromic conjugated polymer. Journal of Polymer Science Part A, 2010, 48, 3913-3923.	2.5	20

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73	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, 1485-1490.	1.2	20
74	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.	4.0	20
75	Density Functional Theory Study of the Oxidation of Ammonia on the IrO₂(110) Surface. Langmuir, 2011, 27, 14253-14259.	1.6	19
76	Photoisomerization and Photodissociation of m-Xylene in a Molecular Beam. Journal of Physical Chemistry A, 2003, 107, 4019-4024.	1.1	18
77	On the search for Câ€“Hâ€“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.	1.2	17
78	Pressure-Enhanced Câˆ’HÂ·Â·Â·O Interactions in Aqueoustert-Butyl Alcohol. Journal of Physical Chemistry A, 2004, 108, 11001-11005.	1.1	16
79	Local Structures of Water in 1-Butyl-3-methylimidazolium Tetrafluoroborate Probed by High-Pressure Infrared Spectroscopy. Analytical Sciences, 2008, 24, 1305-1309.	0.8	16
80	Conjugated polymers containing electron-deficient main chains and electron-rich pendant groups: Synthesis and application to electroluminescence. Organic Electronics, 2011, 12, 1048-1062.	1.4	16
81	High-Pressure Raman Studies on Aqueous Protonated Thiazole:Â Presence of Charge-Enhanced Câˆ’HÂ·Â·Â·O Hydrogen Bonds. Journal of Physical Chemistry B, 2005, 109, 23103-23107.	1.2	15
82	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, 883-888.	1.2	15
83	Amide-containing zinc(ii) metalâ€“organic layered networks: a structureâ€“CO2 capture relationship. Inorganic Chemistry Frontiers, 2015, 2, 477-484.	3.0	15
84	Effects of the terminal donor unit in dyes with Dâ€“Dâ€“Ïâ€“A architecture on the regeneration mechanism in DSSCs: a computational study. Physical Chemistry Chemical Physics, 2018, 20, 23564-23577.	1.3	15
85	On the Search for H₅O₂⁺centered Water Clusters in the Gas Phase. Journal of the Chinese Chemical Society, 1999, 46, 427-434.	0.8	14
86	Microkinetic Simulation of Temperature-Programmed Desorption. Journal of Physical Chemistry C, 2013, 117, 6136-6142.	1.5	14
87	Amide-CO₂Interaction Induced Gate-Opening Behavior for CO₂Adsorption in 2-Fold Interpenetrating Framework. ChemistrySelect, 2016, 1, 2923-2929.	0.7	14
88	Temperature-programmed desorption studies of NH3 and H2O on the RuO2(110) surface: effects of adsorbate diffusion. Physical Chemistry Chemical Physics, 2018, 20, 24201-24209.	1.3	14
89	Proton-Assisted Hydration at Hydrophobic Sites in Protonated Ether and Keto Dimers. Journal of Physical Chemistry A, 1999, 103, 8753-8761.	1.1	13
90	Synthesis and computational oxidation mechanism study of novel organosoluble aramids with high modulus by lowâ€temperature solution polycondensation. Journal of Polymer Science Part A, 2010, 48, 5659-5669.	2.5	13

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91	Density Functional Theory Study of Ethanol Decomposition on 3Ni/Î±-Al₂O₃(0001) Surface. Langmuir, 2010, 26, 15845-15851.	1.6	13
92	Neutrally colourless, transparent and thermally stable polynorbornenes via ring-opening metathesis polymerisation for near-infrared electroactive applications. Journal of Materials Chemistry, 2011, 21, 8597.	6.7	13
93	High-Purity Semiconducting Single-Walled Carbon Nanotubes via Selective Dispersion in Solution Using Fully Conjugated Polytriarylamines. Macromolecules, 2016, 49, 8520-8529.	2.2	13
94	New Insights into Organic Dye Regeneration Mechanism in Dye-Sensitized Solar Cells: A Theoretical Study. ACS Sustainable Chemistry and Engineering, 2017, 5, 8619-8629.	3.2	13
95	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.	0.5	12
96	Characterization of extraframework aluminum in H-mordenite dealuminated with ammonium hexafluorosilicate. Catalysis Today, 2004, 97, 13-23.	2.2	12
97	The role of charge-enhanced Câ€“Hâ‹¯O interactions in gel-like mixtures prepared from ionic liquids and tungsten(VI) oxide nanoparticles. Chemical Physics Letters, 2006, 427, 310-316.	1.2	12
98	Theoretical study on molecular design and optical properties of organic sensitizers. Physical Chemistry Chemical Physics, 2014, 16, 15389.	1.3	12
99	Theoretical insight into hydroxyl production via H₂O₂ decomposition over the Fe₃O₄(311) surface. RSC Advances, 2021, 11, 36257-36264.	1.7	12
100	Enhancement of chlorobenzene sensing by doping aluminum on nanotubes: A DFT study. Applied Surface Science, 2020, 514, 145897.	3.1	11
101	Prediction of SEI Formation in Allâ€Solidâ€State Batteries: Computational Insights from PCLâ€based Polymer Electrolyte Decomposition on Lithiumâ€Metal. Batteries and Supercaps, 2022, 5, .	2.4	11
102	Initial growth of chemical-vapor-deposited Ru from bis(hexafluoroacetylacetonate)dicarbonyl ruthenium. Thin Solid Films, 2005, 483, 31-37.	0.8	10
103	Surface Raman Spectroscopy of trans-Stilbene on Ag/Ge(111): Surface-Induced Effects. Journal of Physical Chemistry C, 2009, 113, 208-212.	1.5	10
104	Preparation of neutrally colorless, transparent polynorbornenes with multiple redoxâ€active chromophores via ringâ€opening metathesis polymerization toward electrochromic applications. Journal of Polymer Science Part A, 2011, 49, 3248-3259.	2.5	10
105	Density Functional Theory Study of Water-Gas-Shift Reaction on 3Cu/Î±-Al2O3(0001) Surface. Journal of Physical Chemistry C, 2013, 117, 12045-12053.	1.5	10
106	Pressure-enhanced surface interactions between nano-TiO₂ and ionic liquid mixtures probed by high pressure IR spectroscopy. Physical Chemistry Chemical Physics, 2015, 17, 21143-21148.	1.3	10
107	Reduction mechanism of iron titanium based oxygen carriers with H₂for chemical looping applications â€“ a combined experimental and theoretical study. RSC Advances, 2016, 6, 106340-106346.	1.7	10
108	Adsorption and Decomposition of Ethylene Carbonate on LiMn2O4 Cathode Surface. Electrochimica Acta, 2016, 210, 61-70.	2.6	10

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109	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.	1.0	10
110	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.	0.8	10
111	A computational study of CO oxidation on IrO2 (1 1 0) surface. Applied Surface Science, 2021, 539, 148244.	3.1	10
112	Direct visualization of lattice oxygen evolution and related electronic properties of Li1.2Ni0.2Mn0.6O2 cathode materials. Applied Surface Science, 2021, 563, 150334.	3.1	10
113	Pressure-dependent studies on hydration of the Câ€“H group in formic acid. Journal of Chemical Physics, 2001, 115, 8032-8037.	1.2	9
114	DFT study on dissociative adsorption of SiH4 and GeH4 on SiGe(100)-2Ã—1 surface. Surface Science, 2006, 600, 3194-3201.	0.8	9
115	Mechanism of Growth of the Ge Wetting Layer Upon Exposure of Si(100)-2 Ã— 1 to GeH4. Journal of the American Chemical Society, 2008, 130, 5440-5442.	6.6	9
116	Effect of solvent proton affinity on the kinetics of michael addition polymerization of n ,n â€²-bismaleimide-4,4â€²-diphenylmethane with barbituric acid. Polymer Engineering and Science, 2014, 54, 559-568.	1.5	9
117	B, Nâ€coâ€doped grapheneâ€supported Ir and Pt clusters for methane activation and Câ”€C coupling: A density functional theory study. Journal of Computational Chemistry, 2020, 41, 194-202.	1.5	9
118	A first-principles study on double-sided decorated boronâ€“nitrogen co-doped graphene by vanadium for enhanced low-temperature reversible hydrogen storage. Sustainable Energy and Fuels, 2021, 5, 2159-2168.	2.5	9
119	Comparable catalytic activity of a low-cost catalyst IrO2/TiO2 for methane conversion â€“ A density functional theory study. Applied Surface Science, 2022, 577, 151938.	3.1	9
120	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.	1.5	9
121	The effect of pressure on charge-enhanced Câ€“Hâ‹¯O interactions in aqueous triethylamine hydrochloride probed by high pressure Raman spectroscopy. Chemical Physics Letters, 2006, 432, 100-105.	1.2	8
122	Energetics and Rate Constants of Si₂H₆ and Ge₂H₆ Dissociative Adsorption on Dimers of SiGe(100)-2 Ã— 1. Journal of Physical Chemistry C, 2007, 111, 13466-13472.	1.5	8
123	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.	1.5	8
124	Quantum Chemical Studies of Methane Oxidation to Methanol on a Biomimetic Tricopper Complex: Mechanistic Insights. ChemistrySelect, 2018, 3, 5113-5122.	0.7	8
125	Theoretical Study of Electrochemical and Electrochromic Properties of Novel Viologen Derivatives: Effects of Donors and Ï€-Conjugation. Journal of Physical Chemistry B, 2019, 123, 4735-4744.	1.2	8
126	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.	1.5	8

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127	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.	2.1	8
128	A first principles study of H₂S adsorption and decomposition on a Ge(100) surface. RSC Advances, 2015, 5, 3825-3832.	1.7	7
129	Theoretical study on the interaction of iodide electrolyte/organic dye with the TiO₂ surface in dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2020, 22, 26410-26418.	1.3	7
130	Tuning Interfacial Thermal and Electrical Conductance across a Metal/MoS₂ Monolayer through Nâ€Methylâ€2â€pyrrolidone Wet Cleaning. Advanced Materials Interfaces, 2020, 7, 2000364.	1.9	7
131	Specific interactions between the quaternary ammonium oligoether-based ionic liquid and water as a function of pressure. Physical Chemistry Chemical Physics, 2013, 15, 12734.	1.3	6
132	A theoretical design of some silole-based dibenzothiophene-S,S-dioxide semiconducting compounds for red phosphorescence. Organic Electronics, 2018, 54, 270-276.	1.4	6
133	Theoretical study on wetting behavior of B-SWNT: Effects of doping concentration. Applied Surface Science, 2019, 497, 143798.	3.1	6
134	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.	1.5	6
135	Silole and selenophene-based D-Ï€-A dyes in dye-sensitized solar cells: Insights from optoelectronic and regeneration properties. Dyes and Pigments, 2020, 176, 108243.	2.0	6
136	The fluorescence turn-off mechanism of a norbornene-derived homopolymer â€“ an Al³⁺ colorimetric and fluorescent chemosensor. Materials Advances, 0, , .	2.6	6
137	Intermolecular Interactions in Aqueous Dimethyl Sulphoxide and Acetic Acid Probed by Highâ€Pressure FTIR. Journal of the Chinese Chemical Society, 2002, 49, 663-667.	0.8	5
138	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, 565-575.	1.3	5
139	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.	0.8	5
140	The investigation of methane storage at the Ni-MOF-74 material: a periodic DFT calculation. Physical Chemistry Chemical Physics, 2021, 23, 12270-12279.	1.3	5
141	Theoretical investigation of CO2 conversion on corrugated g-C3N4 Surface decorated by single-atom of Fe, Co, and Pd. Molecular Catalysis, 2022, 526, 112402.	1.0	5
142	Study of Pathway of Hydrogen Migration and Desorption on SiGe(100) Surface UsingAb InitioCalculations. Japanese Journal of Applied Physics, 2005, 44, 7625-7633.	0.8	4
143	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.	1.5	4
144	Spin-polarized transport properties in some transition metal dithiolene complexes. Physical Chemistry Chemical Physics, 2017, 19, 32536-32543.	1.3	4

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145	Effects of hydrogen on GaN metalorganic vapor-phase epitaxy using tertiarybutylhydrazine as nitrogen source. Journal of Crystal Growth, 2004, 266, 347-353.	0.7	3
146	Photodissociation and photoisomerization of Î±-fluorotoluene and 4-fluorotoluene in a molecular beam. Journal of Chemical Physics, 2006, 125, 133305.	1.2	3
147	Hydrophobic hydration in aqueous acetic acid and formic acid solutions probed by high pressure. Journal of Luminescence, 2002, 98, 177-182.	1.5	2
148	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.	2.4	2
149	Molecular Bending: An Important Factor Affecting the Packing of Self-Assembled Monolayers of Triptycene-Based Molecular Rods on a (111) Gold Surface. Journal of Physical Chemistry C, 2022, 126, 7193-7207.	1.5	2
150	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.	0.8	1
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