Jer-Lai Kuo

List of Publications by Citations

196 papers	6,766 citations	45 h-index	74 g-index
205 ext. papers	7,477 ext. citations	4.5 avg, IF	6.13 L-index

#	Paper	IF	Citations
196	Raman spectroscopy of epitaxial graphene on a SiC substrate. *Physical Review B*, **2008**, 77,	3.3	429
195	Adsorption and diffusion of Li on pristine and defective graphene. *ACS Applied Materials & Interfaces*, **2012**, 4, 2432-8	9.5	300
194	Orbital analysis of electronic structure and phonon dispersion in MoS2, MoSe2, WS2, and WSe2 monolayers under strain. *Physical Review B*, **2013**, 88,	3.3	260
193	Opening an electrical band gap of bilayer graphene with molecular doping. *ACS Nano*, **2011**, 5, 7517-24	16.7	191
192	Band gap opening of graphene by doping small boron nitride domains. *Nanoscale*, **2012**, 4, 2157-65	7.7	190
191	Adsorption of single Li and the formation of small Li clusters on graphene for the anode of lithium-ion batteries. *ACS Applied Materials & Interfaces*, **2013**, 5, 7793-7	9.5	156
190	Theoretical Prediction of Anode Materials in Li-Ion Batteries on Layered Black and Blue Phosphorus. *Journal of Physical Chemistry C*, **2015**, 119, 8662-8670	3.8	147
189	Protonated clathrate cages enclosing neutral water molecules: (H+)(H2O)21 and (H+)(H2O)28. *Journal of Chemical Physics*, **2005**, 122, 074315	3.9	139
188	High-Sulfur-Vacancy Amorphous Molybdenum Sulfide as a High Current Electrocatalyst in Hydrogen Evolution. *Small*, **2016**, 12, 5530-5537	11	138
187	Spin-orbit splitting in single-layer MoS2 revealed by triply resonant Raman scattering. *Physical Review Letters*, **2013**, 111, 126801	7.4	117
186	Metallic VS2 Monolayer Polytypes as Potential Sodium-Ion Battery Anode via ab Initio Random Structure Searching. *ACS Applied Materials & Interfaces*, **2016**, 8, 18754-62	9.5	110
185	Stacking-Dependent Interlayer Coupling in Trilayer MoS with Broken Inversion Symmetry. *Nano Letters*, **2015**, 15, 8155-61	11.5	106
184	On the use of graph invariants for efficiently generating hydrogen bond topologies and predicting physical properties of water clusters and ice. *Journal of Chemical Physics*, **2001**, 114, 2527-2540	3.9	103
183	DFT Study of Hydrogen Storage by Spillover on Graphene with Boron Substitution. *Journal of Physical Chemistry C*, **2011**, 115, 9241-9249	3.8	102
182	Density and Phonon-Stiffness Anomalies of Water and Ice in the Full Temperature Range. *Journal of Physical Chemistry Letters*, **2013**, 4, 3238-44	6.4	101
181	Recent advances in understanding the structures of medium-sized protonated water clusters. *International Reviews in Physical Chemistry*, **2005**, 24, 553-578	7	97
180	A first-principles examination of conducting monolayer 1T'-MX (M = Mo, W; X = S, Se, Te): promising catalysts for hydrogen evolution reaction and its enhancement by strain. *Physical Chemistry Chemical Physics*, **2015**, 17, 21702-8	3.6	95

179	Structure of protonated water clusters: low-energy structures and finite temperature behavior. *Journal of Chemical Physics*, **2005**, 122, 024516	3.9	93
178	Metal free hydrogenation reaction on carbon doped boron nitride fullerene: A DFT study on the kinetic issue. *International Journal of Hydrogen Energy*, **2012**, 37, 14336-14342	6.7	82
177	Density functional study on ferromagnetism in nitrogen-doped anatase TiO2. *Applied Physics Letters*, **2009**, 95, 062505	3.4	81
176	Vibrational predissociation spectra and hydrogen-bond topologies of H+(H2O)9-11. *Physical Chemistry Chemical Physics*, **2005**, 7, 938-44	3.6	78
175	Short H-bonds and spontaneous self-dissociation in (H2O)20: Effects of H-bond topology. *Journal of Chemical Physics*, **2003**, 118, 3583-3588	3.9	78
174	Hydrogen-bond topology and the ice VII/VIII and ice Ih/XI proton-ordering phase transitions. *Physical Review Letters*, **2005**, 94, 135701	7.4	78
173	The Electronic Properties of Single-Layer and Multilayer MoS2 under High Pressure. *Journal of Physical Chemistry C*, **2015**, 119, 10189-10196	3.8	73
172	Band Gap Tuning of Graphene by Adsorption of Aromatic Molecules. *Journal of Physical Chemistry C* , **2012**, 116, 13788-13794	3.8	73
171	High-Pressure-Induced Comminution and Recrystallization of CH NH PbBr Nanocrystals as Large Thin Nanoplates. *Advanced Materials*, **2018**, 30, 1705017	24	73
170	Structural trends of ionized water networks: Infrared spectroscopy of watercluster radical cations (H2O)n+ (n = 3–11). *Chemical Science*, **2011**, 2, 868-876	9.4	72
169	Pressure-Engineered Structural and Optical Properties of Two-Dimensional (CHNH)PbI Perovskite Exfoliated nm-Thin Flakes. *Journal of the American Chemical Society*, **2019**, 141, 1235-1241	16.4	61
168	A first-principle analysis on the phase stabilities, chemical bonds and band gaps of wurtzite structure A(x)Zn(1-x)O alloys (A = Ca, Cd, Mg). *Journal of Physics Condensed Matter*, **2008**, 20, 235221	1.8	60
167	Stereocontrolled intramolecular aziridination of glycals: ready access to aminoglycosides and mechanistic insights from DFT studies. *Chemistry - A European Journal*, **2008**, 14, 1561-70	4.8	59
166	Phase evolution of lithium intercalation dynamics in 2H-MoS. *Nanoscale*, **2017**, 9, 7533-7540	7.7	58
165	First-principles study on ferromagnetism in nitrogen-doped In2O3. *Applied Physics Letters*, **2009**, 95, 012509	3.4	57
164	Li adsorption, hydrogen storage and dissociation using monolayer MoS2: an ab initio random structure searching approach. *Physical Chemistry Chemical Physics*, **2015**, 17, 11367-74	3.6	56
163	A direct first principles study on the structure and electronic properties of BexZn1−xO. *Applied Physics Letters*, **2007**, 91, 121121	3.4	56
162	A Hierarchical Approach to Study the Thermal Behavior of Protonated Water Clusters H(+)(H2O)n. *Journal of Chemical Theory and Computation*, **2009**, 5, 2629-39	6.4	55

161	Hydrogen bond topology and the ice VII/VIII and Ih/XI proton ordering phase transitions. *Physical Review E*, **2006**, 73, 056113	2.4	55
160	Oxygen reduction reaction on active sites of heteroatom-doped graphene. *RSC Advances*, **2013**, 3, 5498	3.7	54
159	Interaction between graphene and the surface of SiO2. *Journal of Physics Condensed Matter*, **2012**, 24, 305004	1.8	52
158	Density functional theory study of finite carbon chains. *ACS Nano*, **2009**, 3, 3788-94	16.7	52
157	Hydrogen-Bonding Evolution during the Polymorphic Transformations in CH3NH3PbBr3: Experiment and Theory. *Chemistry of Materials*, **2017**, 29, 5974-5981	9.6	51
156	Mechanistic insights into the substrate-controlled stereochemistry of glycals in one-pot rhodium-catalyzed aziridination and aziridine ring opening. *Chemistry - A European Journal*, **2010**, 16, 588-94	4.8	50
155	Energy Transfer from Photo-Excited Fluorene Polymers to Single-Walled Carbon Nanotubes. *Journal of Physical Chemistry C*, **2009**, 113, 14946-14952	3.8	49
154	Defect-Mediated Gold Substitution Doping in ZnO Mesocrystals and Catalysis in CO Oxidation. *ACS Catalysis*, **2016**, 6, 115-122	13.1	48
153	Activating and tuning basal planes of MoO_2, MoS_2 and $MoSe_2$ for hydrogen evolution reaction. *Physical Chemistry Chemical Physics*, **2015**, 17, 29305-10	3.6	47
152	Discriminative generation and hydrogen modulation of the Dirac-Fermi polarons at graphene edges and atomic vacancies. *Carbon*, **2011**, 49, 3615-3621	10.4	46
151	Highly stereoselective synthesis of aminoglycosides via rhodium-catalyzed and substrate-controlled aziridination of glycals. *Organic and Biomolecular Chemistry*, **2009**, 7, 1284-7	3.9	45
150	The effect of proton disorder on the structure of ice-Ih: a theoretical study. *Journal of Chemical Physics*, **2005**, 123, 134505	3.9	44
149	A first principles study on the structure of ice-VI: static distortion, molecular geometry, and proton ordering. *Journal of Physical Chemistry B*, **2006**, 110, 3697-703	3.4	43
148	Structure of Ice-VII and Ice-VIII: A Quantum Mechanical Study *Journal of Physical Chemistry B*, **2004**, 108, 19634-19639	3.4	43
147	Assessment of density functional approximations for the hemibonded structure of the water dimer radical cation. *Physical Chemistry Chemical Physics*, **2012**, 14, 10705-12	3.6	38
146	Carbon doped boron nitride cages as competitive candidates for hydrogen storage materials. *Chemical Communications*, **2010**, 46, 883-5	5.8	38
145	Functionalizing Single- and Multi-layer Graphene with Br and Br2. *Journal of Physical Chemistry C*, **2010**, 114, 14939-14945	3.8	38
144	Graphene nanoribbon band-gap expansion: broken-bond-induced edge strain and quantum entrapment. *Nanoscale*, **2010**, 2, 2160-3	7.7	37

143	A theoretical study of thermal stability and electronic properties of wurtzite and zincblende ZnOxS1⊠. *New Journal of Physics*, **2009**, 11, 093008	2.9	37
142	Probing hydrophilic interface of solid/liquid-water by nanoultrasonics. *Scientific Reports*, **2014**, 4, 6249	4.9	36
141	Anisotropy of electron-phonon coupling in single wurtzite CdS nanowires. *Applied Physics Letters*, **2007**, 91, 171911	3.4	36
140	Nuclear quantum effects on the structure and energetics of (H2O)6H+. *Physical Chemistry Chemical Physics*, **2005**, 7, 2324-32	3.6	36
139	Theoretical prediction of hydrogen storage on Li-decorated monolayer black phosphorus. *Journal Physics D: Applied Physics*, **2014**, 47, 465302	3	35
138	Local structure relaxation, quantum trap depression, and valence charge polarization induced by the shorter-and-stronger bonds between under-coordinated atoms in gold nanostructures. *Nanoscale*, **2010**, 2, 412-7	7.7	34
137	Dissociation of hydrogen fluoride in HF(H(2)O)(7). *Journal of Chemical Physics*, **2004**, 120, 4690-5	3.9	34
136	Graph invariants for periodic systems: towards predicting physical properties from the hydrogen bond topology of ice. *Physical Review E*, **2003**, 67, 016114	2.4	34
135	Communication: Trapping a proton in argon: Spectroscopy and theory of the proton-bound argon dimer and its solvation. *Journal of Chemical Physics*, **2016**, 145, 231101	3.9	34
134	Exploration of hydrogen bond networks and potential energy surfaces of methanol clusters using a two-stage clustering algorithm. *Physical Chemistry Chemical Physics*, **2016**, 19, 544-556	3.6	33
133	High pressure photoluminescence and Raman investigations of CdSe⊠nS core/shell quantum dots. *Applied Physics Letters*, **2007**, 90, 021921	3.4	33
132	Folding of the hydrogen bond network of H(+)(CH3OH)7 with rare gas tagging. *Journal of Physical Chemistry A*, **2013**, 117, 101-7	2.8	31
131	Towards the ionic limit of two-dimensional materials: monolayer alkaline earth and transition metal halides. *Physical Chemistry Chemical Physics*, **2014**, 16, 20763-71	3.6	30
130	Collision-induced dissociation of sodiated glucose and identification of anomeric configuration. *Physical Chemistry Chemical Physics*, **2017**, 19, 15454-15462	3.6	30
129	Electronic structures of graphene/boron nitride sheet superlattices. *Physical Review B*, **2011**, 84,	3.3	30
128	Discovering Unique, Low-Energy Pure Water Isomers: Memetic Exploration, Optimization, and Landscape Analysis. *IEEE Transactions on Evolutionary Computation*, **2010**, 14, 419-437	15.6	29
127	Roles of Cu codoping and oxygen vacancies on ferromagnetism in In2O3:Fe. *Physical Review B*, **2009** , 79,	3.3	28
126	Multiscale approach to explore the potential energy surface of water clusters (H2O)nn . *Journal of Physical Chemistry A*, **2008**, 112, 6257-61	2.8	28

125	Density Functional Study of the First Wetting Layer on the GaN (0001) Surface. *Journal of Physical Chemistry C*, **2013**, 117, 8774-8783	3.8	27
124	Enrichment of (8,4) single-walled carbon nanotubes through coextraction with heparin. *Small*, **2010**, 6, 110-8	11	27
123	Structural evolution and solvation of the OH radical in ionized water radical cations (H2O)n(+), n = 5-8. *Physical Chemistry Chemical Physics*, **2014**, 16, 18888-95	3.6	26
122	Molecular adsorption induces the transformation of rhombohedral- to Bernal-stacking order in trilayer graphene. *Nature Communications*, **2013**, 4, 2074	17.4	26
121	Nonconventional magnetism in pristine and alkali doped In2O3: Density functional study. *Journal of Applied Physics*, **2010**, 108, 093911	2.5	26
120	Compatibility between methanol and water in the three-dimensional cage formation of large-sized protonated methanol-water mixed clusters. *Journal of Chemical Physics*, **2007**, 126, 194306	3.9	26
119	The dynamics and spectroscopic fingerprint of hydroxyl radical generation through water dimer ionization: ab initio molecular dynamic simulation study. *Physical Chemistry Chemical Physics*, **2012**, 14, 13402-8	3.6	25
118	Predicting the hydrogen bond ordered structures of ice Ih, II, III, VI and ice VII: DFT methods with localized based set. *Computational Materials Science*, **2010**, 49, S170-S175	3.2	25
117	The low-temperature proton-ordered phases of ice predicted by ab initio methods. *Physical Chemistry Chemical Physics*, **2005**, 7, 3733-7	3.6	25
116	An ab initio anharmonic approach to study vibrational spectra of small ammonia clusters. *Physical Chemistry Chemical Physics*, **2016**, 18, 30498-30506	3.6	25
115	Structures of hydrogen bond networks formed by a few tens of methanol molecules in the gas phase: size-selective infrared spectroscopy of neutral and protonated methanol clusters. *Physical Chemistry Chemical Physics*, **2013**, 15, 9523-30	3.6	24
114	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
113	Features in Vibrational Spectra Induced by Ar-Tagging for H3O(+)Arm, m = 0-3. *Journal of Physical Chemistry A*, **2015**, 119, 10887-92	2.8	23
112	Theoretical analyses of the morphological development of the hydrogen bond network in protonated methanol clusters. *Journal of Physical Chemistry A*, **2007**, 111, 9438-45	2.8	23
111	Composition-temperature phase diagram of BexZn1⊠O from first principles. *Computational Materials Science*, **2010**, 49, S29-S31	3.2	22
110	On the Use of Bond-Counting Rules in Predicting the Stability of C12B6N6 Fullerene. *Journal of Physical Chemistry C*, **2008**, 112, 15691-15696	3.8	22
109	Structural stability of single-layer MoS2 under large strain. *Journal of Physics Condensed Matter*, **2015**, 27, 105401	1.8	21
108	A possible origin of room temperature ferromagnetism in Indium□tin oxide thin film: Surface spin polarization and ferromagnetism. *Physica B: Condensed Matter*, **2011**, 406, 3166-3169	2.8	21

107	Modulation of electronic properties from stacking orders and spin-orbit coupling for 3R-type MoS2. *Scientific Reports*, **2016**, 6, 24140	4.9	21
106	Pressure-Induced Phase Transition in Weyl Semimetallic WTe. *Small*, **2017**, 13, 1701887	11	20
105	Assessment of density functional theory to calculate the phase transition pressure of ice. *Physical Chemistry Chemical Physics*, **2012**, 14, 11484-90	3.6	20
104	First-principles study of the magnetization of oxygen-depleted In(2)O(3)(001) surfaces. *Journal of Physics Condensed Matter*, **2009**, 21, 272202	1.8	20
103	Tuning the vibrational coupling of HO by changing its solvation environment. *Physical Chemistry Chemical Physics*, **2016**, 18, 30721-30732	3.6	19
102	Fermi resonance in solvated HO: a counter-intuitive trend confirmed via a joint experimental and theoretical investigation. *Physical Chemistry Chemical Physics*, **2018**, 20, 13836-13844	3.6	19
101	Effects of X (V, W, Mo, Hf, Ta, Zr) additions on the ideal cleavage fracture of Cr2Nb: First-principles determination. *Intermetallics*, **2010**, 18, 65-69	3.5	19
100	A new layer compound Nb4SiC3predicted from first-principles theory. *Journal Physics D: Applied Physics*, **2009**, 42, 075404	3	19
99	A first-principle study on the structure, stability and hardness of cubic BC2N. *Diamond and Related Materials*, **2009**, 18, 1278-1282	3.5	19
98	Collision-induced dissociation of sodiated glucose, galactose, and mannose, and the identification of anomeric configurations. *Physical Chemistry Chemical Physics*, **2018**, 20, 19614-19624	3.6	18
97	Comprehensive analysis of the hydrogen bond network morphology and OH stretching vibrations in protonated methanol-water mixed clusters, H(+)(MeOH)1(H2O)n (n = 1-8). *Journal of Physical Chemistry A*, **2008**, 112, 10125-33	2.8	18
96	Hydrogen-bonded ring closing and opening of protonated methanol clusters H(+)(CH3OH)(n) (n = 4-8) with the inert gas tagging. *Physical Chemistry Chemical Physics*, **2015**, 17, 22042-53	3.6	17
95	Vibrational spectra of small methylamine clusters accessed by an ab initio anharmonic approach. *Physical Chemistry Chemical Physics*, **2018**, 20, 7653-7660	3.6	17
94	Anticooperative effect induced by mixed solvation in H+ (CH3OH)m(H2O)n (m + n = 5 and 6): a theoretical and infrared spectroscopic study. *Journal of Physical Chemistry A*, **2010**, 114, 8170-7	2.8	17
93	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
92	Temperature dependent structural variations of OH(-)(H2O)n, n = 4-7: effects on vibrational and photoelectron spectra. *Physical Chemistry Chemical Physics*, **2015**, 17, 19162-72	3.6	16
91	An infrared spectroscopic and theoretical study on (CH3)3N-H(+)-(H2O)(n), n = 1-22: highly polarized hydrogen bond networks of hydrated clusters. *Physical Chemistry Chemical Physics*, **2015**, 17, 25863-76	3.6	16
90	Strong Quantum Coupling in the Vibrational Signatures of a Symmetric Ionic Hydrogen Bond: The Case of (CH3OH)2H(.). *Journal of Physical Chemistry A*, **2015**, 119, 11320-8	2.8	16

89	First principles molecular dynamics study of filled ice hydrogen hydrate. *Journal of Chemical Physics*, **2012**, 137, 084505	3.9	16
88	Unveiling the crystallographic facet dependence of the photoelectrochemical glycerol oxidation on bismuth vanadate. *Applied Catalysis B: Environmental*, **2020**, 278, 119303	21.8	15
87	Hydrogen bond induced enhancement of Fermi resonances in N-HN hydrogen bonded complexes of anilines. *Physical Chemistry Chemical Physics*, **2018**, 20, 21557-21566	3.6	14
86	Structural and Electronic Properties of Monolayer 1T-MoS2 Phase, and Its Interaction with Water Adsorbed on Perfect, Single S-Vacated and MoS2-Unit-Vacated Surface: Density Functional Theory Calculations. *Integrated Ferroelectrics*, **2014**, 156, 93-101	0.8	14
85	Proton location in (CH3)3N-H+-(CH3OH)n: A theoretical and infrared spectroscopic study. *Chemical Physics*, **2013**, 421, 1-9	2.3	14
84	Structures and dissociation channels of protonated mixed clusters around a small magic number: infrared spectroscopy of ((CH3)3N)n-H(+)-H2O (n = 1-3). *Journal of Physical Chemistry A*, **2012**, 116, 6740-9	2.8	14
83	Possible room temperature ferromagnetism of Li-doped anatase TiO2: A first-principles study. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2010**, 374, 4451-4454	2.3	14
82	Visualization and investigation of Si□ covalent bonding of single carbon nanotube grown on silicon substrate. *Applied Physics Letters*, **2008**, 93, 103111	3.4	14
81	IR-VUV spectroscopy of pyridine dimers, trimers and pyridine-ammonia complexes in a supersonic jet. *Physical Chemistry Chemical Physics*, **2020**, 22, 21520-21534	3.6	14
80	A closer examination of the coupling between ionic hydrogen bond (IHB) stretching and flanking group motions in (CH3OH)2H(+): the strong isotope effects. *Physical Chemistry Chemical Physics*, **2016**, 18, 14531-42	3.6	14
79	Infrared spectra and anharmonic coupling of proton-bound nitrogen dimers N-H-N, N-D-N, and N-H-N in solid para-hydrogen. *Physical Chemistry Chemical Physics*, **2017**, 19, 20484-20492	3.6	13
78	Infrared spectra of neutral dimethylamine clusters: An infrared-vacuum ultraviolet spectroscopic and anharmonic vibrational calculation study. *Journal of Chemical Physics*, **2019**, 150, 064317	3.9	12
77	A theoretical study on the infrared signatures of proton-bound rare gas dimers (Rg-H-Rg), Rg = {Ne, Ar, Kr, and Xe}. *Journal of Chemical Physics*, **2019**, 150, 124305	3.9	12
76	Unexpected Dissociation Mechanism of Sodiated N-Acetylglucosamine and N-Acetylgalactosamine. *Journal of Physical Chemistry A*, **2019**, 123, 3441-3453	2.8	12
75	Tunable Gravimetric and Volumetric Hydrogen Storage Capacities in Polyhedral Oligomeric Silsesquioxane Frameworks. *ACS Applied Materials & Interfaces*, **2016**, 8, 25219-28	9.5	12
74	Structure prediction of the solid forms of methanol: an ab initio random structure searching approach. *Physical Chemistry Chemical Physics*, **2016**, 18, 2736-46	3.6	12
73	Comprehensive analysis on the structure and proton switch in H+ (CH3OH)m(H2O)n (m + n = 5 and 6). *Journal of Physical Chemistry A*, **2010**, 114, 3096-102	2.8	12
72	Theoretical study of the structural and electronic properties of SimGen and SimGen- (s = m + n . *Journal of Physical Chemistry A*, **2008**, 112, 2235-41	2.8	12

71	EVOLUTIONARY DISCOVERY OF TRANSITION STATES IN WATER CLUSTERS. *Journal of Theoretical and Computational Chemistry*, **2012**, 11, 965-995	1.8	11
70	Proton switch correlated with the morphological development of the hydrogen-bond network in H+ (MeOH)m(H2O)1 (m = 1-9): a theoretical and infrared spectroscopic study. *Journal of Physical Chemistry A*, **2009**, 113, 2323-32	2.8	11
69	Phonon and elastic instabilities in rocksalt calcium oxide under pressure: a first-principles study. *Journal of Physics Condensed Matter*, **2009**, 21, 015402	1.8	11
68	On the effects of basis-set in studying the hydration and dissociation of HF in cubic HF(H2O)7 clusters. *Chemical Physics Letters*, **2008**, 453, 13-17	2.5	11
67	Hydrogen bond network structures of protonated short-chain alcohol clusters. *Physical Chemistry Chemical Physics*, **2018**, 20, 14971-14991	3.6	10
66	First principles studies on the redox ability of (Ga(1-x)Zn(x))N(1-x)O(x) solid solutions and thermal reactions for H2 and O2 production on their surfaces. *Physical Chemistry Chemical Physics*, **2013**, 15, 19807-18	3.6	10
65	Structural and Dynamic Properties of Water on the GaN Polar Surface. *Journal of Physical Chemistry C*, **2011**, 115, 22444-22450	3.8	10
64	Physisorption Structure of Water on the GaN Polar Surface: Force Field Development and Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2011**, 115, 11684-11693	3.8	10
63	Infrared photodissociation spectroscopy and density-functional calculations of protonated methanol cluster ions: Solvation structures of an excess proton. *Journal of Chemical Physics*, **2008**, 129, 084304	3.9	10
62	A liquid crucible model for aggregation of phenylacetylene in the gas phase. *Physical Chemistry Chemical Physics*, **2019**, 21, 13623-13632	3.6	9
61	Tetrahedral Silsesquioxane Framework: A Feasible Candidate for Hydrogen Storage. *Journal of Physical Chemistry C*, **2015**, 119, 23820-23829	3.8	9
60	Strong Fermi Resonance Associated with Proton Motions Revealed by Vibrational Spectra of Asymmetric Proton-Bound Dimers. *Angewandte Chemie - International Edition*, **2021**, 60, 1936-1941	16.4	9
59	Stepwise Internal Energy Change of Protonated Methanol Clusters By Using the Inert Gas Tagging. *Journal of Physical Chemistry A*, **2016**, 120, 9203-9208	2.8	8
58	Polar ordering and structural distortion in electronic domain-wall properties of BiFeO3. *Journal of Applied Physics*, **2017**, 122, 075103	2.5	8
57	First-principles study of band gap engineering of ZnO by alloying with LiGaO2 for ultraviolet applications. *Journal of Applied Physics*, **2013**, 114, 063715	2.5	8
56	Feature Selection Using Single/Multi-Objective Memetic Frameworks. *Studies in Computational Intelligence*, **2009**, 111-131	0.8	8
55	Hydrogen enhancing Ga doping efficiency and electron mobility in high-performance transparent conducting Ga-doped ZnO films. *Journal of Alloys and Compounds*, **2021**, 860, 158518	5.7	8
54	Deconstructing Vibrational Motions on the Potential Energy Surfaces of Hydrogen-Bonded Complexes. *CCS Chemistry*, **2021**, 3, 829-835	7.2	8

53	Vibrational spectroscopic signatures of hydrogen bond induced NH stretch-bend Fermi-resonance in amines: The methylamine clusters and other N-H?N hydrogen-bonded complexes. *Journal of Chemical Physics*, **2020**, 153, 194301	3.9	7
52	Vibrational spectroscopy of protonated amine-water clusters: tuning Fermi resonance and lighting up dark states. *Physical Chemistry Chemical Physics*, **2020**, 22, 22035-22046	3.6	7
51	Toward Closing the Gap between Hexoses and -Acetylhexosamines: Experimental and Computational Studies on the Collision-Induced Dissociation of Hexosamines. *Journal of Physical Chemistry A*, **2019**, 123, 6683-6700	2.8	6
50	Calculation of near K edge x-ray absorption spectra and hydrogen bond network in ice XIII under compression. *Journal of Chemical Physics*, **2010**, 132, 184506	3.9	6
49	First principle study on the structure of H+(H2O)6. *Journal of Physics: Conference Series*, **2006**, 28, 87-90	0.3	6
48	Multilevel Approach for Direct VSCF/VCI MULTIMODE Calculations with Applications to Large "Zundel" Cations. *Journal of Chemical Theory and Computation*, **2018**, 14, 6405-6416	6.4	6
47	Spin-charge-lattice coupling in YBaCuFeO: Optical properties and first-principles calculations. *Scientific Reports*, **2019**, 9, 3223	4.9	5
46	Mechanistic Insight on the Formation of a Solid Electrolyte Interphase (SEI) by an Acetonitrile-Based Superconcentrated [Li][TFSI] Electrolyte near Lithium Metal. *Journal of Physical Chemistry C*, **2020**, 124, 27495-27502	3.8	5
45	Microscopic evidence for the dissociation of water molecules on cleaved GaN(11[combining macron]00). *Physical Chemistry Chemical Physics*, **2018**, 20, 1261-1266	3.6	5
44	Removal of Water Adsorbates on GaN Surfaces via Hopping Processes and with the Aid of a Pt4 Cluster: An Ab Initio Study. *Journal of Physical Chemistry C*, **2014**, 118, 20383-20392	3.8	5
43	Temperature and Size Dependence of Characteristic Hydrogen-Bonded Network Structures with Ion Core Switching in Protonated (Methanol)-(Water) Mixed Clusters: A Revisit. *Journal of Physical Chemistry A*, **2017**, 121, 5399-5413	2.8	5
42	The role of sp-hybridized atoms in carbon ferromagnetism: a spin-polarized density functional theory calculation. *Journal of Physics Condensed Matter*, **2010**, 22, 046001	1.8	5
41	Vibrational Coupling in Solvated HO: Interplay between Fermi Resonance and Combination Band. *Journal of Physical Chemistry Letters*, **2020**, 11, 10067-10072	6.4	5
40	Structure and Vibrational Spectra of ArH (= 2-3). *Journal of Physical Chemistry A*, **2020**, 124, 7726-7734	2.8	5
39	Direct enumeration of wurtzite BC2N configurations for structural stability and hardness evaluation. *Diamond and Related Materials*, **2010**, 19, 100-105	3.5	4
38	Finding multiple first order saddle points using a valley adaptive clearing genetic algorithm **2009**,		4
37	Theoretical Study on Structural Stability of Alloy Cages: a Case of Silicon-doped Heterofullerenes. *Communications in Computational Physics*, **2010**, 8, 289-303	2.4	4
36	Hydrogen roles approaching ideal electrical and optical properties for undoped and Al doped ZnO thin films. *Journal of Materiomics*, **2021**,	6.7	4

35	Competition between hydrogen bonds and van der Waals forces in intermolecular structure formation of protonated branched-chain alcohol clusters. *Physical Chemistry Chemical Physics*, **2018**, 20, 25482-25494	3.6	4
34	DFT Study on the H2 Storage Properties of Sc-Decorated Covalent Organic Frameworks Based on Adamantane Units. *Journal of Physical Chemistry C*, **2018**, 122, 16853-16865	3.8	4
33	Effects of mixing between short-chain and branched-chain alcohols in protonated clusters. *Physical Chemistry Chemical Physics*, **2020**, 22, 13223-13239	3.6	3
32	Graphene homojunction: closed-edge bilayer graphene by pseudospin interaction. *Nanoscale*, **2016**, 8, 9102-6	7.7	3
31	A LAMMPS implementation of volume□emperature replica exchange molecular dynamics. *Computer Physics Communications*, **2015**, 189, 119-127	4.2	3
30	Structure and vibrational spectra of H(+)(HF)(n) (n=2-9) clusters: An ab initio study. *Journal of Chemical Physics*, **2009**, 131, 224307	3.9	3
29	Hydrogen adsorption mechanism of MOF-74 metal-organic frameworks: an insight from first principles calculations.. *RSC Advances*, **2020**, 10, 43940-43949	3.7	3
28	Anharmonic coupling behind vibrational spectra of solvated ammonium: lighting up overtone states by Fermi resonance through tuning solvation environments. *Physical Chemistry Chemical Physics*, **2020**, 22, 24059-24069	3.6	3
27	Dipole moment enhanced □stacking in fluorophenylacetylenes is carried over from gas-phase dimers to crystal structures propagated through liquid like clusters. *Physical Chemistry Chemical Physics*, **2021**, 23, 9938-9947	3.6	3
26	Collision-induced dissociation of xylose and its applications in linkage and anomericity identification. *Physical Chemistry Chemical Physics*, **2021**, 23, 3485-3495	3.6	3
25	Vibrational Signature of Dynamic Coupling of a Strong Hydrogen Bond. *Journal of Physical Chemistry Letters*, **2021**, 12, 2259-2265	6.4	3
24	Improved agreement between experimental and computational results for collision-induced dissociation mass spectrometry of cation-tagged hexoses. *Physical Chemistry Chemical Physics*, **2020**, 22, 6928-6941	3.6	2
23	Proton Quantum Confinement on Symmetric Dimers of Ammonia and Lower Amine Homologs. *Progress in Theoretical Chemistry and Physics*, **2015**, 77-89	0.6	2
22	From the perspectives of DFT calculations, thermodynamic modeling, and kinetic Monte Carlo simulations: the interaction between hydrogen and ScC monolayers. *Physical Chemistry Chemical Physics*, **2020**, 22, 4387-4401	3.6	2
21	Fermi resonance switching in KrHRg and XeHRg (Rg = Ne, Ar, Kr, and Xe). *Journal of Chemical Physics*, **2021**, 154, 134302	3.9	2
20	The Spectroscopic Features of Ionized Water Medium: Theoretical Characterization and Implication Using (H2O)n+, n=3□4, Cluster Model. *Journal of the Chinese Chemical Society*, **2016**, 63, 488-498	1.5	2
19	Lithium and sodium intercalation in a 2D NbSe bilayer-stacked homostructure: comparative study of ionic adsorption and diffusion behavior. *Physical Chemistry Chemical Physics*, **2021**, 23, 19811-19818	3.6	2
18	Understanding Fermi resonances in the complex vibrational spectra of the methyl groups in methylamines. *Physical Chemistry Chemical Physics*, **2021**, 23, 3739-3747	3.6	2

17	Size of the hydrogen bond network in liquid methanol: a quantum cluster equilibrium model with extensive structure search. *Physical Chemistry Chemical Physics*, **2021**, 23, 9166-9175	3.6	2
16	The natural valence band offset of dilute GaAs1−xNx and GaAs: The first-principles approach. *Computational Materials Science*, **2010**, 49, S150-S152	3.2	1
15	Mechano-chemical stability and water effect on gas selectivity in mixed-metal zeolitic imidazolate frameworks: a systematic investigation from van der Waals corrected density functional theory. *Physical Chemistry Chemical Physics*, **2020**, 22, 1598-1610	3.6	1
14	The electronic structures and magnetic properties of mixed-valence Fe-based metal-organic VNU-15 frameworks: a theoretical study from linear response DFT+U calculations.. *RSC Advances*, **2020**, 10, 34690-34701	3.7	1
13	Anharmonic Coupling Revealed by the Vibrational Spectra of Solvated Protonated Methanol: Fermi Resonance, Combination Bands, and Isotope Effect. *Journal of Physical Chemistry A*, **2021**, 125, 1910-1918	2.8	1
12	Is Dissociation of HCl in DMSO Clusters Bistable?. *Journal of Physical Chemistry A*, **2021**, 125, 10351-10358	2.8	0
11	An anharmonic approach to IR, Raman and SFG spectra of the solvated methylammonium ion. *Physical Chemistry Chemical Physics*, **2021**, 23, 25736-25747	3.6	0
10	Disentangling the Complex Vibrational Spectra of Hydrogen-Bonded Clusters of 2-Pyridone with Structural Search and Anharmonic Analysis. *Journal of Physical Chemistry A*, **2021**, 125, 4306-4312	2.8	0
9	Infrared Spectroscopy and Anharmonic Vibrational Analysis of (HO-Kr) (= 1-3): Hemibond Formation of the Water Radical Cation. *Journal of Physical Chemistry Letters*, **2021**, 12, 7997-8002	6.4	0
8	Structures of Pyridine-Water Clusters Studied with Infrared-Vacuum Ultraviolet Spectroscopy. *Journal of Physical Chemistry A*, **2021**, 125, 7489-7501	2.8	0
7	A decomposition mechanism for Mn(DSBDC) metal-organic frameworks in the presence of water molecules. *Physical Chemistry Chemical Physics*, **2021**, 23, 22794-22803	3.6	0
6	Spectral Signatures of Protonated Noble Gas Clusters of Ne, Ar, Kr, and Xe: From Monomers to Trimers. *Molecules*, **2022**, 27, 3198	4.8	0
5	Distinct reactivities on segmented selenium nanorods. *Chemical Communications*, **2015**, 51, 13783-6	5.8	
4	Quantum-mechanical approach to predissociation of water dimers in the vibrational adiabatic representation: Importance of channel interactions. *Journal of Chemical Physics*, **2015**, 143, 084303	3.9	
3	Structural and vibrational characterization of HCO and Rg-HCO, Rg = {He, Ne, Ar, Kr, and Xe}. *Journal of Chemical Physics*, **2021**, 155, 174306	3.9	
2	Why is the Donor-Acceptor Stretching a sine qua non in Understanding the Vibrational Signatures of Ionic Hydrogen Bonds?. *Progress in Theoretical Chemistry and Physics*, **2017**, 251-269	0.6	
1	Strong Fermi Resonance Associated with Proton Motions Revealed by Vibrational Spectra of Asymmetric Proton-Bound Dimers. *Angewandte Chemie*, **2021**, 133, 1964-1969	3.6	