Jer-Lai Kuo

List of Publications by Year in Descending Order

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	Spectral Signatures of Protonated Noble Gas Clusters of Ne, Ar, Kr, and Xe: From Monomers to Trimers. *Molecules*, **2022**, 27, 3198	4.8	0
195	Is Dissociation of HCl in DMSO Clusters Bistable?. *Journal of Physical Chemistry A*, **2021**, 125, 10351-10358	2.8	0
194	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	
193	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
192	Fermi resonance switching in KrHRg and XeHRg (Rg = Ne, Ar, Kr, and Xe). *Journal of Chemical Physics*, **2021**, 154, 134302	3.9	2
191	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
190	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
189	Hydrogen roles approaching ideal electrical and optical properties for undoped and Al doped ZnO thin films. *Journal of Materiomics*, **2021**,	6.7	4
188	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
187	Strong Fermi Resonance Associated with Proton Motions Revealed by Vibrational Spectra of Asymmetric Proton-Bound Dimers. *Angewandte Chemie*, **2021**, 133, 1964-1969	3.6	
186	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
185	Collision-induced dissociation of xylose and its applications in linkage and anomericity identification. *Physical Chemistry Chemical Physics*, **2021**, 23, 3485-3495	3.6	3
184	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
183	Vibrational Signature of Dynamic Coupling of a Strong Hydrogen Bond. *Journal of Physical Chemistry Letters*, **2021**, 12, 2259-2265	6.4	3
182	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
181	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
180	Structures of Pyridine-Water Clusters Studied with Infrared-Vacuum Ultraviolet Spectroscopy. *Journal of Physical Chemistry A*, **2021**, 125, 7489-7501	2.8	0

179	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
178	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
177	Deconstructing Vibrational Motions on the Potential Energy Surfaces of Hydrogen-Bonded Complexes. *CCS Chemistry*, **2021**, 3, 829-835	7.2	8
176	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
175	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
174	Effects of mixing between short-chain and branched-chain alcohols in protonated clusters. *Physical Chemistry Chemical Physics*, **2020**, 22, 13223-13239	3.6	3
173	Unveiling the crystallographic facet dependence of the photoelectrochemical glycerol oxidation on bismuth vanadate. *Applied Catalysis B: Environmental*, **2020**, 278, 119303	21.8	15
172	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
171	Hydrogen adsorption mechanism of MOF-74 metal-organic frameworks: an insight from first principles calculations.. *RSC Advances*, **2020**, 10, 43940-43949	3.7	3
170	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
169	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
168	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
167	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
166	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
165	Vibrational Coupling in Solvated HO: Interplay between Fermi Resonance and Combination Band. *Journal of Physical Chemistry Letters*, **2020**, 11, 10067-10072	6.4	5
164	Structure and Vibrational Spectra of ArH (= 2-3). *Journal of Physical Chemistry A*, **2020**, 124, 7726-7734	2.8	5
163	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
162	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

161	A liquid crucible model for aggregation of phenylacetylene in the gas phase. *Physical Chemistry Chemical Physics*, **2019**, 21, 13623-13632	3.6	9
160	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
159	Spin-charge-lattice coupling in YBaCuFeO: Optical properties and first-principles calculations. *Scientific Reports*, **2019**, 9, 3223	4.9	5
158	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
157	Unexpected Dissociation Mechanism of Sodiated N-Acetylglucosamine and N-Acetylgalactosamine. *Journal of Physical Chemistry A*, **2019**, 123, 3441-3453	2.8	12
156	Toward Closing the Gap between Hexoses and -Acetlyhexosamines: Experimental and Computational Studies on the Collision-Induced Dissociation of Hexosamines. *Journal of Physical Chemistry A*, **2019**, 123, 6683-6700	2.8	6
155	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
154	Hydrogen bond network structures of protonated short-chain alcohol clusters. *Physical Chemistry Chemical Physics*, **2018**, 20, 14971-14991	3.6	10
153	Vibrational spectra of small methylamine clusters accessed by an ab initio anharmonic approach. *Physical Chemistry Chemical Physics*, **2018**, 20, 7653-7660	3.6	17
152	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
151	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
150	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
149	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
148	High-Pressure-Induced Comminution and Recrystallization of CH NH PbBr Nanocrystals as Large Thin Nanoplates. *Advanced Materials*, **2018**, 30, 1705017	24	73
147	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
146	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
145	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
144	Phase evolution of lithium intercalation dynamics in 2H-MoS. *Nanoscale*, **2017**, 9, 7533-7540	7.7	58

143	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
142	Hydrogen-Bonding Evolution during the Polymorphic Transformations in CH3NH3PbBr3: Experiment and Theory. *Chemistry of Materials*, **2017**, 29, 5974-5981	9.6	51
141	Polar ordering and structural distortion in electronic domain-wall properties of BiFeO3. *Journal of Applied Physics*, **2017**, 122, 075103	2.5	8
140	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
139	Collision-induced dissociation of sodiated glucose and identification of anomeric configuration. *Physical Chemistry Chemical Physics*, **2017**, 19, 15454-15462	3.6	30
138	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
137	Pressure-Induced Phase Transition in Weyl Semimetallic WTe. *Small*, **2017**, 13, 1701887	11	20
136	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	
135	High-Sulfur-Vacancy Amorphous Molybdenum Sulfide as a High Current Electrocatalyst in Hydrogen Evolution. *Small*, **2016**, 12, 5530-5537	11	138
134	Tunable Gravimetric and Volumetric Hydrogen Storage Capacities in Polyhedral Oligomeric Silsesquioxane Frameworks. *ACS Applied Materials & Interfaces*, **2016**, 8, 25219-28	9.5	12
133	Tuning the vibrational coupling of HO by changing its solvation environment. *Physical Chemistry Chemical Physics*, **2016**, 18, 30721-30732	3.6	19
132	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
131	Graphene homojunction: closed-edge bilayer graphene by pseudospin interaction. *Nanoscale*, **2016**, 8, 9102-6	7.7	3
130	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
129	Defect-Mediated Gold Substitution Doping in ZnO Mesocrystals and Catalysis in CO Oxidation. *ACS Catalysis*, **2016**, 6, 115-122	13.1	48
128	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
127	The Spectroscopic Features of Ionized Water Medium: Theoretical Characterization and Implication Using (H2O)n+, n=3, Cluster Model. *Journal of the Chinese Chemical Society*, **2016**, 63, 488-498	1.5	2
126	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

125	Modulation of electronic properties from stacking orders and spin-orbit coupling for 3R-type MoS2. *Scientific Reports*, **2016**, 6, 24140	4.9	21
124	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
123	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
122	An ab initio anharmonic approach to study vibrational spectra of small ammonia clusters. *Physical Chemistry Chemical Physics*, **2016**, 18, 30498-30506	3.6	25
121	Distinct reactivities on segmented selenium nanorods. *Chemical Communications*, **2015**, 51, 13783-6	5.8	
120	A first-principles examination of conducting monolayer 1T'-MX$_2$ (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
119	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
118	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
117	The Electronic Properties of Single-Layer and Multilayer MoS2 under High Pressure. *Journal of Physical Chemistry C*, **2015**, 119, 10189-10196	3.8	73
116	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
115	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
114	Tetrahedral Silsesquioxane Framework: A Feasible Candidate for Hydrogen Storage. *Journal of Physical Chemistry C*, **2015**, 119, 23820-23829	3.8	9
113	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
112	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	
111	Stacking-Dependent Interlayer Coupling in Trilayer MoS_2 with Broken Inversion Symmetry. *Nano Letters*, **2015**, 15, 8155-61	11.5	106
110	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
109	Structural stability of single-layer MoS2 under large strain. *Journal of Physics Condensed Matter*, **2015**, 27, 105401	1.8	21
108	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

107	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
106	A LAMMPS implementation of volume-temperature replica exchange molecular dynamics. *Computer Physics Communications*, **2015**, 189, 119-127	4.2	3
105	Proton Quantum Confinement on Symmetric Dimers of Ammonia and Lower Amine Homologs. *Progress in Theoretical Chemistry and Physics*, **2015**, 77-89	0.6	2
104	Probing hydrophilic interface of solid/liquid-water by nanoultrasonics. *Scientific Reports*, **2014**, 4, 6249	4.9	36
103	Theoretical prediction of hydrogen storage on Li-decorated monolayer black phosphorus. *Journal Physics D: Applied Physics*, **2014**, 47, 465302	3	35
102	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
101	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
100	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
99	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
98	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
97	Spin-orbit splitting in single-layer MoS2 revealed by triply resonant Raman scattering. *Physical Review Letters*, **2013**, 111, 126801	7.4	117
96	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
95	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
94	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
93	Proton location in (CH3)3N-H+-(CH3OH)n: A theoretical and infrared spectroscopic study. *Chemical Physics*, **2013**, 421, 1-9	2.3	14
92	Oxygen reduction reaction on active sites of heteroatom-doped graphene. *RSC Advances*, **2013**, 3, 5498	3.7	54
91	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
90	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

89	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
88	Molecular adsorption induces the transformation of rhombohedral- to Bernal-stacking order in trilayer graphene. *Nature Communications*, **2013**, 4, 2074	17.4	26
87	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
86	Interaction between graphene and the surface of SiO2. *Journal of Physics Condensed Matter*, **2012**, 24, 305004	1.8	52
85	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
84	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
83	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
82	Band Gap Tuning of Graphene by Adsorption of Aromatic Molecules. *Journal of Physical Chemistry C* , **2012**, 116, 13788-13794	3.8	73
81	Band gap opening of graphene by doping small boron nitride domains. *Nanoscale*, **2012**, 4, 2157-65	7.7	190
80	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
79	First principles molecular dynamics study of filled ice hydrogen hydrate. *Journal of Chemical Physics*, **2012**, 137, 084505	3.9	16
78	Adsorption and diffusion of Li on pristine and defective graphene. *ACS Applied Materials & Interfaces*, **2012**, 4, 2432-8	9.5	300
77	Assessment of density functional theory to calculate the phase transition pressure of ice. *Physical Chemistry Chemical Physics*, **2012**, 14, 11484-90	3.6	20
76	EVOLUTIONARY DISCOVERY OF TRANSITION STATES IN WATER CLUSTERS. *Journal of Theoretical and Computational Chemistry*, **2012**, 11, 965-995	1.8	11
75	DFT Study of Hydrogen Storage by Spillover on Graphene with Boron Substitution. *Journal of Physical Chemistry C*, **2011**, 115, 9241-9249	3.8	102
74	Structural trends of ionized water networks: Infrared spectroscopy of watercluster radical cations (H2O)n+ (n = 3□1). *Chemical Science*, **2011**, 2, 868-876	9.4	72
73	Structural and Dynamic Properties of Water on the GaN Polar Surface. *Journal of Physical Chemistry C*, **2011**, 115, 22444-22450	3.8	10
72	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

71	Opening an electrical band gap of bilayer graphene with molecular doping. *ACS Nano*, **2011**, 5, 7517-24	16.7	191
70	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
69	Discriminative generation and hydrogen modulation of the Dirac-Fermi polarons at graphene edges and atomic vacancies. *Carbon*, **2011**, 49, 3615-3621	10.4	46
68	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
67	Electronic structures of graphene/boron nitride sheet superlattices. *Physical Review B*, **2011**, 84,	3.3	30
66	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
65	Direct enumeration of wurtzite BC2N configurations for structural stability and hardness evaluation. *Diamond and Related Materials*, **2010**, 19, 100-105	3.5	4
64	Carbon doped boron nitride cages as competitive candidates for hydrogen storage materials. *Chemical Communications*, **2010**, 46, 883-5	5.8	38
63	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
62	Graphene nanoribbon band-gap expansion: broken-bond-induced edge strain and quantum entrapment. *Nanoscale*, **2010**, 2, 2160-3	7.7	37
61	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
60	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
59	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
58	Composition-temperature phase diagram of BexZn1□O from first principles. *Computational Materials Science*, **2010**, 49, S29-S31	3.2	22
57	The natural valence band offset of dilute GaAs1□Nx and GaAs: The first-principles approach. *Computational Materials Science*, **2010**, 49, S150-S152	3.2	1
56	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
55	Functionalizing Single- and Multi-layer Graphene with Br and Br2. *Journal of Physical Chemistry C*, **2010**, 114, 14939-14945	3.8	38
54	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

53	Nonconventional magnetism in pristine and alkali doped In2O3: Density functional study. *Journal of Applied Physics*, **2010**, 108, 093911	2.5	26
52	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
51	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
50	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
49	Enrichment of (8,4) single-walled carbon nanotubes through coextraction with heparin. *Small*, **2010**, 6, 110-8	11	27
48	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
47	Finding multiple first order saddle points using a valley adaptive clearing genetic algorithm **2009**,		4
46	Roles of Cu codoping and oxygen vacancies on ferromagnetism in In2O3:Fe. *Physical Review B*, **2009** , 79,	3.3	28
45	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
44	Energy Transfer from Photo-Excited Fluorene Polymers to Single-Walled Carbon Nanotubes. *Journal of Physical Chemistry C*, **2009**, 113, 14946-14952	3.8	49
43	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
42	A theoretical study of thermal stability and electronic properties of wurtzite and zincblende ZnOxS1□. *New Journal of Physics*, **2009**, 11, 093008	2.9	37
41	First-principles study on ferromagnetism in nitrogen-doped In2O3. *Applied Physics Letters*, **2009**, 95, 012509	3.4	57
40	Feature Selection Using Single/Multi-Objective Memetic Frameworks. *Studies in Computational Intelligence*, **2009**, 111-131	0.8	8
39	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
38	Density functional study on ferromagnetism in nitrogen-doped anatase TiO2. *Applied Physics Letters*, **2009**, 95, 062505	3.4	81
37	A new layer compound Nb4SiC3predicted from first-principles theory. *Journal Physics D: Applied Physics*, **2009**, 42, 075404	3	19
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