I-Feng W Kuo

List of Publications by Citations

32 papers	2,086 citations	20 h-index	34 g-index
34 ext. papers	2,223 ext. citations	6.8 avg, IF	4.52 L-index

#	Paper	IF	Citations
32	Liquid Water from First Principles: Investigation of Different Sampling Approaches. *Journal of Physical Chemistry B*, **2004**, 108, 12990-12998	3.4	309
31	An ab initio molecular dynamics study of the aqueous liquid-vapor interface. *Science*, **2004**, 303, 658-60	33.3	299
30	Molecular dynamics simulation of liquid water: hybrid density functionals. *Journal of Physical Chemistry B*, **2006**, 110, 3685-91	3.4	222
29	Dynamic ionization of water under extreme conditions. *Physical Review Letters*, **2005**, 94, 125508	7.4	190
28	Simulating fluid-phase equilibria of water from first principles. *Journal of Physical Chemistry A*, **2006**, 110, 640-6	2.8	125
27	The Effect of Polarizability for Understanding the Molecular Structure of Aqueous Interfaces. *Journal of Chemical Theory and Computation*, **2007**, 3, 2002-10	6.4	107
26	Hydroxide anion at the air-water interface. *Chemical Physics Letters*, **2009**, 481, 2-8	2.5	103
25	Bonding in the superionic phase of water. *Physical Review Letters*, **2005**, 94, 217801	7.4	95
24	Isobaric-isothermal monte carlo simulations from first principles: application to liquid water at ambient conditions. *ChemPhysChem*, **2005**, 6, 1894-901	3.2	93
23	Toward a unified picture of the water self-ions at the air-water interface: a density functional theory perspective. *Journal of Physical Chemistry B*, **2014**, 118, 8364-72	3.4	77
22	Time-Dependent Properties of Liquid Water: A Comparison of Car-Parrinello and Born-Oppenheimer Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2006**, 2, 1274-81	6.4	72
21	First-principles approaches to the structure and reactivity of atmospherically relevant aqueous interfaces. *Chemical Reviews*, **2006**, 106, 1282-304	68.1	66
20	QM/MM metadynamics study of the direct decarboxylation mechanism for orotidine-5-monophosphate decarboxylase using two different QM regions: acceleration too small to explain rate of enzyme catalysis. *Journal of Physical Chemistry B*, **2007**, 111, 12573-81	3.4	52
19	Spectral signatures of the pentagonal water cluster in bacteriorhodopsin. *ChemPhysChem*, **2008**, 9, 2703-12	3.2	31
18	Ultrafast shock initiation of exothermic chemistry in hydrogen peroxide. *Journal of Physical Chemistry A*, **2013**, 117, 13051-8	2.8	29
17	The high pressure structure and equation of state of 2,6-diamino-3,5-dinitropyrazine-1-oxide (LLM-105) up to 20 GPa: X-ray diffraction measurements and first principles molecular dynamics simulations. *Journal of Chemical Physics*, **2015**, 143, 144506	3.9	28
16	Thermal Fluctuations of the Unusually Symmetric and Stable Superoxide Tetrahydrate Complex: An ab Initio Molecular Dynamics Study. *Journal of Physical Chemistry A*, **2002**, 106, 10969-10976	2.8	27

List of Publications

15	HYDROPHOBIC HYDRATION FROM CAR□PARRINELLO SIMULATIONS. *International Journal of Modern Physics B*, **2004**, 18, 1951-1962	1.1	26
14	Toward a Monte Carlo program for simulating vapor□liquid phase equilibria from first principles. *Computer Physics Communications*, **2005**, 169, 289-294	4.2	25
13	First-principles high-pressure unreacted equation of state and heat of formation of crystal 2,6-diamino-3, 5-dinitropyrazine-1-oxide (LLM-105). *Journal of Chemical Physics*, **2014**, 141, 064702	3.9	24
12	Pressure-induced phase transition in 1,3,5-triamino-2,4,6-trinitrobenzene (TATB). *Applied Physics Letters*, **2019**, 114, 191901	3.4	14
11	Migration of positively charged defects in □quartz. *Physical Review B*, **2007**, 76,	3.3	13
10	Effects of pressure on the structure and lattice dynamics of □glycine: a combined experimental and theoretical study. *CrystEngComm*, **2019**, 21, 4457-4464	3.3	12
9	Mechanochemical synthesis of glycine oligomers in a virtual rotational diamond anvil cell. *Chemical Science*, **2020**, 11, 7760-7771	9.4	11
8	Determination of enthalpies of formation of energetic molecules with composite quantum chemical methods. *Chemical Physics Letters*, **2016**, 648, 31-35	2.5	8
7	Determination of the Surface Effects on Sarin Degradation. *Journal of Physical Chemistry C*, **2012**, 116, 9631-9635	3.8	7
6	First-principles molecular dynamics simulations of condensed-phase V-type nerve agent reaction pathways and energy barriers. *Physical Chemistry Chemical Physics*, **2012**, 14, 3316-22	3.6	5
5	High-Pressure Equation of State of 1,3,5-triamino-2,4,6-trinitrobenzene: Insights into the Monoclinic Phase Transition, Hydrogen Bonding, and Anharmonicity. *Journal of Physical Chemistry A* , **2020**, 124, 10580-10591	2.8	5
4	Predicted Reaction Mechanisms, Product Speciation, Kinetics, and Detonation Properties of the Insensitive Explosive 2,6-Diamino-3,5-dinitropyrazine-1-oxide (LLM-105). *Journal of Physical Chemistry A*, **2021**, 125, 1766-1777	2.8	5
3	An Isosymmetric High-Pressure Phase Transition in □Glycylglycine: A Combined Experimental and Theoretical Study. *Journal of Physical Chemistry B*, **2020**, 124, 1-10	3.4	4
2	Preparation and optimization of a diverse workload for a large-scale heterogeneous system **2019**,		2
1	High-Pressure Investigation of 2,4,6-Trinitro-3-bromoanisole (TNBA): Structural Determination and Piezochromism. *Journal of Physical Chemistry C*, **2022**, 126, 1176-1187	3.8	