I-FengÂ W Kuo

List of Publications by Year
in descending order

33 papers	2,345 citations	377584 21 h-index	488211 31 g-index
34 all docs	34 docs citations	34 times ranked	2573 citing authors

#	Article	IF	Citations
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.	1.5	5
2	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.	1.1	19
3	An Isosymmetric High-Pressure Phase Transition in Î±-Glycylglycine: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry B, 2020, 124, 1-10.	1.2	14
4	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.	1.1	16
5	Mechanochemical synthesis of glycine oligomers in a virtual rotational diamond anvil cell. Chemical Science, 2020, 11, 7760-7771.	3.7	21
6	Effects of pressure on the structure and lattice dynamics of Î±-glycine: a combined experimental and theoretical study. CrystEngComm, 2019, 21, 4457-4464.	1.3	16
7	Pressure-induced phase transition in 1,3,5-triamino-2,4,6-trinitrobenzene (TATB). Applied Physics Letters, 2019, 114, .	1.5	34
8	Preparation and optimization of a diverse workload for a large-scale heterogeneous system. , 2019, , .		3
9	Determination of enthalpies of formation of energetic molecules with composite quantum chemical methods. Chemical Physics Letters, 2016, 648, 31-35.	1.2	15
10	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.	1.2	36
11	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.	1.2	36
12	Toward a Unified Picture of the Water Self-Ions at the Airâ€“Water Interface: A Density Functional Theory Perspective. Journal of Physical Chemistry B, 2014, 118, 8364-8372.	1.2	90
13	Ultrafast Shock Initiation of Exothermic Chemistry in Hydrogen Peroxide. Journal of Physical Chemistry A, 2013, 117, 13051-13058.	1.1	33
14	First-principles molecular dynamics simulations of condensed-phase V-type nerve agent reaction pathways and energy barriers. Physical Chemistry Chemical Physics, 2012, 14, 3316.	1.3	6
15	Determination of the Surface Effects on Sarin Degradation. Journal of Physical Chemistry C, 2012, 116, 9631-9635.	1.5	7
16	Hydroxide anion at the airâ€“water interface. Chemical Physics Letters, 2009, 481, 2-8.	1.2	118
17	Spectral Signatures of the Pentagonal Water Cluster in Bacteriorhodopsin. ChemPhysChem, 2008, 9, 2703-2707.	1.0	32
18	QM/MM Metadynamics Study of the Direct Decarboxylation Mechanism for Orotidine-5â€˜-monophosphate Decarboxylase Using Two Different QM Regions:â€‰ Acceleration Too Small To Explain Rate of Enzyme Catalysis. Journal of Physical Chemistry B, 2007, 111, 12573-12581.	1.2	53

#	Article	IF	Citations
19	Migration of positively charged defects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-quartz. Physical Review B, 2007, 76, .	1.1	13
20	The Effect of Polarizability for Understanding the Molecular Structure of Aqueous Interfaces. Journal of Chemical Theory and Computation, 2007, 3, 2002-2010.	2.3	110
21	Time-Dependent Properties of Liquid Water:â€‰ A Comparison of Carâ€'Parrinello and Bornâ€'Oppenheimer Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2006, 2, 1274-1281.	2.3	77
22	Molecular Dynamics Simulation of Liquid Water:Â Hybrid Density Functionalsâ€. Journal of Physical Chemistry B, 2006, 110, 3685-3691.	1.2	242
23	Simulating Fluid-Phase Equilibria of Water from First Principlesâ€. Journal of Physical Chemistry A, 2006, 110, 640-646.	1.1	128
24	First-Principles Approaches to the Structure and Reactivity of Atmospherically Relevant Aqueous Interfaces. Chemical Reviews, 2006, 106, 1282-1304.	23.0	71
25	Isobaric-Isothermal Monte Carlo Simulations from First Principles: Application to Liquid Water at Ambient Conditions. ChemPhysChem, 2005, 6, 1894-1901.	1.0	99
26	Toward a Monte Carlo program for simulating vaporâ€“liquid phase equilibria from first principles. Computer Physics Communications, 2005, 169, 289-294.	3.0	29
27	Dynamic Ionization of Water under Extreme Conditions. Physical Review Letters, 2005, 94, 125508.	2.9	212
28	Bonding in the Superionic Phase of Water. Physical Review Letters, 2005, 94, 217801.	2.9	99
29	HYDROPHOBIC HYDRATION FROM CARâ€“PARRINELLO SIMULATIONS. International Journal of Modern Physics B, 2004, 18, 1951-1962.	1.0	29
30	Liquid Water from First Principles:Â Investigation of Different Sampling Approaches. Journal of Physical Chemistry B, 2004, 108, 12990-12998.	1.2	327
31	An ab Initio Molecular Dynamics Study of the Aqueous Liquid-Vapor Interface. Science, 2004, 303, 658-660.	6.0	325
32	Thermal Fluctuations of the Unusually Symmetric and Stable Superoxide Tetrahydrate Complex: An ab initio Molecular Dynamics Study.. ChemInform, 2003, 34, no.	0.1	0
33	Thermal Fluctuations of the Unusually Symmetric and Stable Superoxide Tetrahydrate Complex:Â An ab Initio Molecular Dynamics Study. Journal of Physical Chemistry A, 2002, 106, 10969-10976.	1.1	30