Xifan Wu

List of Publications by Year
in descending order

53 papers	4,444 citations	230014 27 h-index	198040 52 g-index
53 all docs	53 docs citations	53 times ranked	6296 citing authors

#	Article	IF	Citations
1	Dissolving salt is not equivalent to applying a pressure on water. Nature Communications, 2022, 13, 822.	5.8	41
2	Convert Widespread Paraelectric Perovskite to Ferroelectrics. Physical Review Letters, 2022, 128, .	2.9	5
3	Many-body effects in the X-ray absorption spectra of liquid water. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2201258119.	3.3	11
4	Importance of nuclear quantum effects on the hydration of chloride ion. Physical Review Materials, 2021, 5, .	0.9	11
5	Nuclear quantum effects on the quasiparticle properties of the chloride anion aqueous solution within the GW approximation. Physical Review B, 2021, 104, .	1.1	6
6	Modeling Liquid Water by Climbing up Jacobâ€™s Ladder in Density Functional Theory Facilitated by Using Deep Neural Network Potentials. Journal of Physical Chemistry B, 2021, 125, 11444-11456.	1.2	40
7	Stabilization of Hydroxide Ions at the Interface of a Hydrophobic Monolayer on Water via Reduced Proton Transfer. Physical Review Letters, 2020, 125, 156803.	2.9	21
8	Deep neural network for the dielectric response of insulators. Physical Review B, 2020, 102, .	1.1	60
9	Isotope effects in x-ray absorption spectra of liquid water. Physical Review B, 2020, 102, .	1.1	6
10	Hydration of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msubsup><mml:mrow><mml:mi>NH</mml:mi></mml:mrow><mml:mrow><mml:mn>4</mml:mn><mml:mo> in Water: Bifurcated Hydrogen Bonding Structures and Fast Rotational Dynamics. Physical Review Letters, 2020, 125, 106001.	2.9	17
11	Interface enhanced functionalities in oxide superlattices under mechanical and electric boundary conditions. Npj Computational Materials, 2020, 6, .	3.5	9
12	Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics. 1. Theory, Algorithm, and Performance. Journal of Chemical Theory and Computation, 2020, 16, 3757-3785.	2.3	29
13	Aqueous solvation of the chloride ion revisited with density functional theory: impact of correlation and exchange approximations. Physical Chemistry Chemical Physics, 2020, 22, 10666-10675.	1.3	20
14	Isotope effects in molecular structures and electronic properties of liquid water via deep potential molecular dynamics based on the SCAN functional. Physical Review B, 2020, 102, .	1.1	22
15	Probing ferroelectricity by x-ray absorption spectroscopy in molecular crystals. Physical Review Materials, 2020, 4, .	0.9	4
16	Accessing the Accuracy of Density Functional Theory through Structure and Dynamics of the Waterâ€“Air Interface. Journal of Physical Chemistry Letters, 2019, 10, 4914-4919.	2.1	43
17	First-principles study of the infrared spectrum in liquid water from a systematically improved description of H-bond network. Physical Review B, 2019, 99, .	1.1	27
18	Importance of van der Waals effects on the hydration of metal ions from the Hofmeister series. Journal of Chemical Physics, 2019, 150, 124505.	1.2	11

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19	Structural, electronic, and dynamical properties of liquid water by ab initio molecular dynamics based on SCAN functional within the canonical ensemble. Journal of Chemical Physics, 2018, 148, 164505.	1.2	58
20	Hydroxide diffuses slower than hydronium in water because its solvated structure inhibits correlated proton transfer. Nature Chemistry, 2018, 10, 413-419.	6.6	175
21	Signature of the hydrogen-bonded environment of liquid water in X-ray emission spectra from first-principles calculations. Frontiers of Physics, 2018, 13, 1.	2.4	3
22	Tuning the NÃ©el Temperature of Hexagonal Ferrites by Structural Distortion. Physical Review Letters, 2018, 121, 237203.	2.9	29
23	Electron-Hole Theory of the Effect of Quantum Nuclei on the X-Ray Absorption Spectra of Liquid Water. Physical Review Letters, 2018, 121, 137401.	2.9	35
24	Identification of a functional point defect in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>SrTi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review Materials, 2018, 2, .	0.9	14
25	Effects of biaxial strain on the improper multiferroicity inhâ”LuFeO3films studied using the restrained thermal expansion method. Physical Review B, 2017, 95, .	1.1	14
26	Ab initio theory and modeling of water. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 10846-10851.	3.3	340
27	X-ray absorption of liquid water by advanced ab initio methods. Physical Review B, 2017, 96, .	1.1	11
28	Comparative first-principles studies of prototypical ferroelectric materials by LDA, GGA, and SCAN meta-GGA. Physical Review B, 2017, 96, .	1.1	156
29	Electronic origin of the spin-phonon coupling effect in transition-metal perovskites. Physical Review B, 2017, 96, .	1.1	2
30	Stabilization of Highly Polar<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>BiFeO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Structure: A New Interface Design Route for Enhanced Ferroelectricity in Artificial Perovskite Superlattices. Physical Review X, 2016, 6, .	2.8	16
31	Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional. Nature Chemistry, 2016, 8, 831-836.	6.6	698
32	A systematic study of chloride ion solvation in water using van der Waals inclusive hybrid density functional theory. Molecular Physics, 2015, 113, 2842-2854.	0.8	47
33	General microscopic model of magnetoelastic coupling from first principles. Physical Review B, 2015, 91, .	1.1	22
34	Room temperature multiferroism in CaTcO3 by interface engineering. Computational Materials Science, 2015, 96, 171-177.	1.4	5
35	The individual and collective effects of exact exchange and dispersion interactions on the ab initio structure of liquid water. Journal of Chemical Physics, 2014, 141, 084502.	1.2	276
36	Structural and electronic origin of the magnetic structures in hexagonal<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">LuFeO</mml:mi></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 90, .	1.1	38

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37	AbÂinitioStudies of Ionization Potentials of Hydrated Hydroxide and Hydronium. Physical Review Letters, 2013, 111, 087801.	2.9	25
38	Crystal field splitting and optical bandgap of hexagonal LuFeO3 films. Applied Physics Letters, 2012, 101, .	1.5	51
39	Roles of quantum nuclei and inhomogeneous screening in the x-ray absorption spectra of water and ice. Physical Review B, 2012, 86, .	1.1	53
40	Modeling functional piezoelectricity in perovskite superlattices with competing instabilities. Physical Review B, 2012, 85, .	1.1	13
41	Interface enhancement of spin-polar phonon coupling in perovskite multiferroic superlattices. Europhysics Letters, 2012, 100, 17005.	0.7	7
42	Electronic structure and bonding properties of cobalt oxide in the spinel structure. Physical Review B, 2011, 83, .	1.1	258
43	Interfacial enhancement of ferroelectricity in CaTiO3/BaTiO3superlattices. Physical Review B, 2011, 83, .	1.1	52
44	X-Ray Absorption Signatures of the Molecular Environment in Water and Ice. Physical Review Letters, 2010, 105, 017802.	2.9	85
45	Order-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>N</mml:mi></mml:math>implementation of exact exchange in extended insulating systems. Physical Review B, 2009, 79, .	1.1	171
46	Hybrid density functional calculations of the band gap of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ga</mml:mtext></mml:mrow><mml:mi>x</mml:mi></mml:msub> Physical Review B, 2009, 80, .	1.1	41
47	Predicting Polarization and Nonlinear Dielectric Response of Arbitrary Perovskite Superlattice Sequences. Physical Review Letters, 2008, 101, 087601.	2.9	45
48	Effects of linear and nonlinear piezoelectricity on the electronic properties ofInAsâˆ•GaAsquantum dots. Physical Review B, 2006, 74, .	1.1	135
49	Importance of Second-Order Piezoelectric Effects in Zinc-Blende Semiconductors. Physical Review Letters, 2006, 96, 187602.	2.9	197
50	Wannier-Based Definition of Layer Polarizations in Perovskite Superlattices. Physical Review Letters, 2006, 97, 107602.	2.9	46
51	Systematic treatment of displacements, strains, and electric fields in density-functional perturbation theory. Physical Review B, 2005, 72, .	1.1	675
52	Metric tensor formulation of strain in density-functional perturbation theory. Physical Review B, 2005, 71, .	1.1	260
53	Structural and Dynamic Properties of Solvated Hydroxide and Hydronium Ions in Water from Ab Initio Modeling. Journal of Chemical Physics, 0, , .	1.2	8