Thomas D KÃ¼hne

List of Publications by Year
in descending order

113 papers	5,544 citations	147801 31 h-index	82547 72 g-index
115 all docs	115 docs citations	115 times ranked	5905 citing authors

#	Article	IF	Citations
1	CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations. Journal of Chemical Physics, 2020, 152, 194103.	3.0	1,371
2	Efficient and Accurate Car-Parrinello-like Approach to Born-Oppenheimer Molecular Dynamics. Physical Review Letters, 2007, 98, 066401.	7.8	351
3	Proton transfer through the water gossamer. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 13723-13728.	7.1	320
4	Vibrational Spectroscopy and Dynamics of Water. Chemical Reviews, 2016, 116, 7590-7607.	47.7	300
5	A High-Rate Two-Dimensional Polyarylimide Covalent Organic Framework Anode for Aqueous Zn-Ion Energy Storage Devices. Journal of the American Chemical Society, 2020, 142, 19570-19578.	13.7	232
6	i-PI 2.0: A universal force engine for advanced molecular simulations. Computer Physics Communications, 2019, 236, 214-223.	7.5	220
7	Static and Dynamical Properties of Liquid Water from First Principles by a Novel Carâ^'Parrinello-like Approach. Journal of Chemical Theory and Computation, 2009, 5, 235-241.	5.3	189
8	Electronic signature of the instantaneous asymmetry in the first coordination shell of liquid water. Nature Communications, 2013, 4, 1450.	12.8	176
9	Mixed Grotthuss and Vehicle Transport Mechanism in Proton Conducting Polymers from Ab initio Molecular Dynamics Simulations. Chemistry of Materials, 2011, 23, 1424-1429.	6.7	172
10	Second generation Carâ€“Parrinello molecular dynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 391-406.	14.6	130
11	New Insights into the Structure of the Vapor/Water Interface from Large-Scale First-Principles Simulations. Journal of Physical Chemistry Letters, 2011, 2, 105-113.	4.6	126
12	Ab initioquality neural-network potential for sodium. Physical Review B, 2010, 81, .	3.2	115
13	Nature of the Asymmetry in the Hydrogen-Bond Networks of Hexagonal Ice and Liquid Water. Journal of the American Chemical Society, 2014, 136, 3395-3399.	13.7	64
14	Energy transfer within the hydrogen bonding network of water following resonant terahertz excitation. Science Advances, 2020, 6, eaay7074.	10.3	62
15	Structure and Dynamics of the Instantaneous Water/Vapor Interface Revisited by Path-Integral and Ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2015, 119, 10079-10086.	2.6	61
16	Covalency of hydrogen bonds in liquid water can be probed by proton nuclear magnetic resonance experiments. Nature Communications, 2015, 6, 8318.	12.8	61
17	Vibrational dynamics in lead halide hybrid perovskites investigated by Raman spectroscopy. Physical Chemistry Chemical Physics, 2020, 22, 5604-5614.	2.8	61
18	On the absolute thermodynamics of water from computer simulations: A comparison of first-principles molecular dynamics, reactive and empirical force fields. Journal of Chemical Physics, 2012, 137, 244507.	3.0	59

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19	Interfacial Covalent Bonds Regulated Electronâ€Deficient 2D Black Phosphorus for Electrocatalytic Oxygen Reactions. Advanced Materials, 2021, 33, e2008752.	21.0	56
20	Microscopic properties of liquid water from combined ab initio molecular dynamics and energy decomposition studies. Physical Chemistry Chemical Physics, 2013, 15, 15746.	2.8	55
21	Evidence for the existence of Li₂S₂ clusters in lithiumâ€“sulfur batteries: ab initio Raman spectroscopy simulation. Physical Chemistry Chemical Physics, 2015, 17, 22009-22014.	2.8	54
22	Vibrational Signature of Water Molecules in Asymmetric Hydrogen Bonding Environments. Journal of Physical Chemistry Letters, 2013, 4, 3245-3250.	4.6	46
23	Quantum Monte Carlo study of high pressure solid molecular hydrogen. New Journal of Physics, 2013, 15, 113005.	2.9	45
24	On the Hydrogen Bond Strength and Vibrational Spectroscopy of Liquid Water. Scientific Reports, 2018, 8, 16888.	3.3	44
25	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.	4.6	43
26	Electrochemical N₂ Reduction to Ammonia Using Single Au/Fe Atoms Supported on Nitrogen-Doped Porous Carbon. ACS Applied Energy Materials, 2020, 3, 10061-10069.	5.1	40
27	Surface tension of ab initio liquid water at the water-air interface. Journal of Chemical Physics, 2016, 144, 204705.	3.0	39
28	An efficient and accurate decomposition of the Fermi operator. Journal of Chemical Physics, 2008, 129, 024707.	3.0	35
29	First-principles study of the amorphous In<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>SbTe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math> phase change compound. Physical Review B, 2013, 88, .	3.2	34
30	Nuclear quantum effects in liquid water from path-integral simulations using anab initioforce-matching approach. Molecular Physics, 2015, 113, 808-822.	1.7	32
31	Database Screening of Ternary Chalcogenides for P-type Transparent Conductors. Chemistry of Materials, 2018, 30, 6794-6800.	6.7	32
32	Quantum ring-polymer contraction method: Including nuclear quantum effects at no additional computational cost in comparison toab initiomolecular dynamics. Physical Review E, 2016, 93, 043305.	2.1	31
33	Photocatalytic Water Splitting Reaction Catalyzed by Ion-Exchanged Salts of Potassium Poly(heptazine) Tj ETQq1 1 0.784314 rgBT /Ov	3.1	30
34	Time-resolved terahertzâ€“Raman spectroscopy reveals that cations and anions distinctly modify intermolecular interactions of water. Nature Chemistry, 2022, 14, 1031-1037.	13.6	29
35	Controlling the strength of interaction between carbon dioxide and nitrogen-rich carbon materials by molecular design. Sustainable Energy and Fuels, 2019, 3, 2819-2827.	4.9	28
36	â€œOn-the-flyâ€•coupled cluster path-integral molecular dynamics: impact of nuclear quantum effects on the protonated water dimer. Physical Chemistry Chemical Physics, 2015, 17, 14355-14359.	2.8	27

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37	Nuclear quantum effects on the vibrational dynamics of liquid water. Journal of Chemical Physics, 2018, 148, 102328.	3.0	27
38	Rational design of transparent p-type conducting non-oxide materials from high-throughput calculations. Journal of Materials Chemistry C, 2018, 6, 541-549.	5.5	27
39	On the role of interfacial hydrogen bonds in â€œon-waterâ€•catalysis. Journal of Chemical Physics, 2014, 141, 22D528.	3.0	26
40	Opposing Electronic and Nuclear Quantum Effects on Hydrogen Bonds in H₂O and D₂O. ChemPhysChem, 2019, 20, 2461-2465.	2.1	25
41	Disordered crystals from first principles I: Quantifying the configuration space. Annals of Physics, 2018, 391, 120-149.	2.8	23
42	Diffusion of Alkali Metals in Polycrystalline CuInSe₂ and Their Role in the Passivation of Grain Boundaries. ACS Applied Materials & Interfaces, 2019, 11, 14821-14829.	8.0	23
43	Impact of intermolecular vibrational coupling effects on the sum-frequency generation spectra of the water/air interface. Molecular Physics, 2020, 118, 1620358.	1.7	22
44	Superionic Conduction in Substoichiometric LiAl Alloy: AnAbÂInitioStudy. Physical Review Letters, 2009, 103, 125901.	7.8	21
45	Modulation of nearly free electron states in hydroxyl-functionalized MXenes: a first-principles study. Journal of Materials Chemistry C, 2020, 8, 5211-5221.	5.5	21
46	Time-dependent vibrational sum-frequency generation spectroscopy of the air-water interface. Communications Chemistry, 2019, 2, .	4.5	20
47	Self-consistent field theory based molecular dynamics with linear system-size scaling. Journal of Chemical Physics, 2014, 140, 134109.	3.0	18
48	Mixedâ€Valence Compounds as Polarizing Agents for Overhauser Dynamic Nuclear Polarization in Solids**. Angewandte Chemie - International Edition, 2021, 60, 15371-15375.	13.8	18
49	Ni-based electrocatalysts for unconventional CO2 reduction reaction to formic acid. Nano Energy, 2022, 97, 107191.	16.0	17
50	Towards electronic structure-based ab-initio molecular dynamics simulations with hundreds of millions of atoms. Parallel Computing, 2022, 111, 102920.	2.1	17
51	First principles simulation of amorphous InSb. Physical Review B, 2013, 87, .	3.2	16
52	Nuclear quantum effects induce metallization of dense solid molecular hydrogen. Journal of Computational Chemistry, 2018, 39, 262-268.	3.3	16
53	Properties of Coâ€Evaporated RbInSe₂ Thin Films. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1800564.	2.4	16
54	Artificial Neural Networks as Trial Wave Functions for Quantum Monte Carlo. Advanced Theory and Simulations, 2021, 4, 2000269.	2.8	16

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55	Anharmonicity and finite-temperature effects on the structure, stability, and vibrational spectrum of phase III of solid molecular hydrogen. Physical Review B, 2014, 90, .	3.2	15
56	Density functional theory study of self-trapped holes in disorderedSiO2. Physical Review B, 2009, 80, .	3.2	14
57	Optimal calculation of the pair correlation function for an orthorhombic system. Physical Review E, 2013, 87, 045301.	2.1	14
58	Efficient â€œOnâ€theâ€Flyâ€•calculation of Raman Spectra from Abâ€Initio molecular dynamics: Application to hydrophobic/hydrophilic solutes in bulk water. Journal of Computational Chemistry, 2015, 36, 2188-2192.	3.3	14
59	High-pressure hydrogen sulfide by diffusion quantum Monte Carlo. Journal of Chemical Physics, 2017, 146, 084503.	3.0	14
60	Sign problem of the fermionic shadow wave function. Physical Review E, 2014, 90, 053304.	2.1	13
61	Competing factors on the frequency separation between the OH stretching modes in water. Journal of Molecular Liquids, 2015, 205, 42-45.	4.9	13
62	Guanine condensates as covalent materials and the concept of cryptopores. Carbon, 2021, 172, 497-505.	10.3	13
63	Enhancement of the local asymmetry in the hydrogen bond network of liquid water by an ultrafast electric field pulse. Scientific Reports, 2019, 9, 10002.	3.3	12
64	Alkali Atoms Diffusion Mechanism in CuInSe₂ Explained by Kinetic Monte Carlo Simulations. Advanced Theory and Simulations, 2019, 2, 1900036.	2.8	12
65	Artificial neural networks for the kinetic energy functional of non-interacting fermions. Journal of Chemical Physics, 2021, 154, 074107.	3.0	12
66	A Hybrid Approach to Fermi Operator Expansion. , 2009, , .		11
67	Assessing the accuracy of improved forceâ€matched water models derived from Ab initio molecular dynamics simulations. Journal of Computational Chemistry, 2016, 37, 1828-1838.	3.3	11
68	Organic Mixed-Valence Compounds and the Overhauser Effect in Insulating Solids. Journal of Physical Chemistry A, 2021, 125, 867-874.	2.5	11
69	Inverse simulated annealing for the determination of amorphous structures. Physical Review B, 2013, 87, .	3.2	10
70	Unconventional phase III of high-pressure solid hydrogen. Physical Review B, 2019, 100, .	3.2	10
71	The effect of Ag, Pb and Bi impurities on grain boundary sliding and intergranular decohesion in Copper. Philosophical Magazine, 2016, 96, 2868-2886.	1.6	9
72	On the Possibility of Helium Adsorption in Nitrogen Doped Graphitic Materials. Scientific Reports, 2020, 10, 5832.	3.3	9

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73	CENT2: Improved charge equilibration via neural network technique. Physical Review B, 2022, 105, .	3.2	9
74	On fermionic shadow wave functions for strongly correlated multi-reference systems based on a single Slater determinant. Europhysics Letters, 2015, 110, 20011.	2.0	8
75	Influence of the exchange and correlation functional on the structure of amorphous InSb and In3SbTe2 compounds. Journal of Chemical Physics, 2016, 144, 204508.	3.0	8
76	Theoretical Investigation of the Interaction of the CuInSe₂ Absorber Material with Oxygen, Hydrogen, and Water. Journal of Physical Chemistry C, 2018, 122, 21202-21209.	3.1	8
77	Correlating facet orientation, defect-level density and dipole layer formation at the surface of polycrystalline CuInSe2 thin films. Acta Materialia, 2020, 200, 463-470.	7.9	8
78	When water becomes an integral part of carbon â€“ combining theory and experiment to understand the zeolite-like water adsorption properties of porous C₂N materials. Journal of Materials Chemistry A, 2021, 9, 22563-22572.	10.3	8
79	An automated approach for developing neural network interatomic potentials with FLAME. Computational Materials Science, 2021, 197, 110567.	3.0	8
80	Resonating valence bond quantum Monte Carlo: Application to the ozone molecule. International Journal of Quantum Chemistry, 2015, 115, 1673-1677.	2.0	7
81	Manyâ€body dispersion interactions for periodic systems based on maximally localized Wannier functions: Application to graphene/water systems. Physica Status Solidi (B): Basic Research, 2016, 253, 308-313.	1.5	7
82	â€œOn-The-Flyâ€•Calculation of the Vibrational Sum-Frequency Generation Spectrum at the Air-Water Interface. Molecules, 2020, 25, 3939.	3.8	7
83	Hydrogen bond dynamics of interfacial water molecules revealed from two-dimensional vibrational sum-frequency generation spectroscopy. Scientific Reports, 2021, 11, 2456.	3.3	6
84	A Massively Parallel Algorithm for the Approximate Calculation of Inverse p-th Roots of Large Sparse Matrices. , 2018, , .		5
85	Impact of finiteâ€temperature and condensedâ€phase effects on theoretical Xâ€ray absorption spectra of transition metal complexes. Journal of Computational Chemistry, 2019, 40, 712-716.	3.3	5
86	Vibrational Properties of RbInSe₂: Raman Scattering Spectroscopy and First-Principle Calculations. Journal of Physical Chemistry C, 2020, 124, 1285-1291.	3.1	5
87	Water structure near the surface of Weyl semimetals as catalysts in photocatalytic proton reduction. Structural Dynamics, 2020, 7, 034101.	2.3	5
88	Accurate Sampling with Noisy Forces from Approximate Computing. Computation, 2020, 8, 39.	2.0	5
89	Tumbling with a limp: local asymmetry in water's hydrogen bond network and its consequences. Physical Chemistry Chemical Physics, 2020, 22, 10397-10411.	2.8	5
90	Thermodynamically stable polymorphs of nitrogen-rich carbon nitrides: a C₃N₅ study. Physical Chemistry Chemical Physics, 2021, 23, 6422-6432.	2.8	5

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91	Equation of state of atomic solid hydrogen by stochastic many-body wave function methods. Journal of Chemical Physics, 2020, 153, 204107.	3.0	5
92	A General Algorithm to Calculate the Inverse Principal p-th Root of Symmetric Positive Definite Matrices. Communications in Computational Physics, 2019, 25, .	1.7	5
93	Second-harmonic generation in atomically thin <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mn>1</mml:mn><mml:mi>T</mml:mi><mml:mtext>â€“</mml:mtext><mml:m and its possible origin from charge density wave transitions. Physical Review B, 2022, 105, .	â€“	5
94	The Structure of Water in Silica Mesopores â€“ Influence of the Pore Wall Polarity. Advanced Materials Interfaces, 2022, 9, .	3.7	5
95	Improved parameterization of the quantum harmonic oscillator model based on localized wannier functions to describe Van der Waals interactions in density functional theory. International Journal of Quantum Chemistry, 2016, 116, 1160-1165.	2.0	4
96	Linear-scaling self-consistent field theory based molecular dynamics: application to C₆₀buckyballs colliding with graphite. Molecular Simulation, 2018, 44, 1380-1386.	2.0	4
97	Disordered crystals from first principles II: Transport coefficients. Annals of Physics, 2020, 421, 168290.	2.8	4
98	Metal-Insulator Transition of Solid Hydrogen by the Antisymmetric Shadow Wave Function. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2018, 73, 845-858.	1.5	3
99	In silicoinvestigation of Cu(In,Ga)Se₂-based solar cells. Physical Chemistry Chemical Physics, 2020, 22, 26682-26701.	2.8	3
100	Oxidation/reduction cycles and their reversible effect on the dipole formation at CuInSe2 surfaces. Physical Review Materials, 2020, 4, .	2.4	3
101	Influence of different ester side groups in polymers on the vapor phase infiltration with trimethyl aluminum. Dalton Transactions, 2022, 51, 1384-1394.	3.3	3
102	Electronic Structures of Group IIIâ€“V Element Haeckelite Compounds: A Novel Family of Semiconductors, Dirac Semimetals, and Topological Insulators. Advanced Functional Materials, 0, , 2110930.	14.9	3
103	Surface Passivation and Detrimental Heat-Induced Diffusion Effects in RbF-Treated Cu(In,Ga)Se₂ Solar Cell Absorbers. ACS Applied Materials & Interfaces, 2022, 14, 34101-34112.	8.0	3
104	Tetraedrisch, wenn flÃ¼ssig. Nachrichten Aus Der Chemie, 2013, 61, 1203-1206.	0.0	2
105	Inverse simulated annealing: Improvements and application to amorphous InSb. Computational Materials Science, 2016, 117, 7-14.	3.0	2
106	Using Approximate Computing for the Calculation of Inverse Matrix <inline-formula> <tex-math notation="LaTeX">p </tex-math> </inline-formula>th Roots. IEEE Embedded Systems Letters, 2018, 10, 33-36.	1.9	2
107	Analysis of sequence-defined oligomers through Advanced Polymer Chromatographyâ„¢ â€“ mass spectrometry hyphenation. RSC Advances, 2020, 10, 35245-35252.	3.6	2
108	Insight from energy decomposition analysis on a hydrogen-bond-mediated mechanism for on-water catalysis. Molecular Physics, 2020, 118, e1797920.	1.7	2

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109	Full Assignment of Ab-Initio Raman Spectra at Finite Temperatures Using Wannier Polarizabilities: Application to Cyclohexane Molecule in Gas Phase. Micromachines, 2021, 12, 1212.	2.9	2
110	A Submatrix-Based Method for Approximate Matrix Function Evaluation in the Quantum Chemistry Code CP2K. , 2020, , .		2
111	Hybrid functional calculations on the Na and K impurities in substitutional and interstitial positions in Cu2ZnSnSe4. , 2015, , .		1
112	Gemischtvalente Verbindungen als polarisierende Mittel fÃ¼r die dynamische Kernâ€Overhauserâ€Polarisation in FestkÃ¶rpern**. Angewandte Chemie, 2021, 133, 15499-15503.	2.0	0
113	Ni-Based Electrocatalysts for Unconventional CO2 Reduction Reaction to Formic Acid. , 0, , .		0