Hsin-Yu Ko

List of Publications by Year
in descending order

21	6,133	516710 16	713466 21
papers	citations	h-index	g-index

21	21	21	8489
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	1.8	4,303
2	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	1.1	445
3	Ab initio theory and modeling of water. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 10846-10851.	7.1	340
4	Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies. Chemical Reviews, 2022, 122, 6117-6321.	47.7	195
5	Hydroxide diffuses slower than hydronium in water because its solvated structure inhibits correlated proton transfer. Nature Chemistry, 2018, 10, 413-419.	13.6	175
6	Free energy of proton transfer at the waterâ€“TiO₂ interface from ab initio deep potential molecular dynamics. Chemical Science, 2020, 11, 2335-2341.	7.4	134
7	Reliable and practical computational description of molecular crystal polymorphs. Science Advances, 2019, 5, eaau3338.	10.3	127
8	Structure, Polarization, and Sum Frequency Generation Spectrum of Interfacial Water on Anatase TiO₂. Journal of Physical Chemistry Letters, 2018, 9, 6716-6721.	4.6	70
9	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.	3.0	58
10	Isotope effects in liquid water via deep potential molecular dynamics. Molecular Physics, 2019, 117, 3269-3281.	1.7	52
11	Expeditious synthesis of aromatic-free piperidinium-functionalized polyethylene as alkaline anion exchange membranes. Chemical Science, 2021, 12, 3898-3910.	7.4	47
12	Local-order metric for condensed-phase environments. Physical Review B, 2018, 97, .	3.2	41
13	Structural properties of water confined by phospholipid membranes. Frontiers of Physics, 2018, 13, 1.	5.0	34
14	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.	5.3	29
15	Root-growth of boron nitride nanotubes: experiments and ab initio simulations. Nanoscale, 2018, 10, 22223-22230.	5.6	19
16	Thermal expansion in dispersion-bound molecular crystals. Physical Review Materials, 2018, 2, .	2.4	18
17	Competitive Adsorption as a Route to Area-Selective Deposition. ACS Applied Materials & Interfaces, 2020, 12, 9989-9999.	8.0	14
18	Hydrogen Dynamics in Supercritical Water Probed by Neutron Scattering and Computer Simulations. Journal of Physical Chemistry Letters, 2020, 11, 9461-9467.	4.6	11

#	Article	IF	Citations
19	Molecular Split-Ring Resonators Based on Metal String Complexes. Journal of Physical Chemistry C, 2014, 118, 3766-3773.	3.1	10
20	Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory-Based Ab Initio Molecular Dynamics II: Extensions to the Isobaricâ€“Isoenthalpic and Isobaricâ€“Isothermal Ensembles. Journal of Chemical Theory and Computation, 2021, 17, 7789-7813.	5.3	7
21	Probing ferroelectricity by x-ray absorption spectroscopy in molecular crystals. Physical Review Materials, 2020, 4, .	2.4	4