Qi Yu

List of Publications by Year in descending order

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30	1,103	394421	477307
papers	citations	19 h-index	29 g-index

30	30	30	998
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Permutationally Invariant Potential Energy Surfaces. Annual Review of Physical Chemistry, 2018, 69, 151-175.	10.8	152
2	Crossover from hydrogen to chemical bonding. Science, 2021, 371, 160-164.	12.6	123
3	Structure, Anharmonic Vibrational Frequencies, and Intensities of NNHNN⁺. Journal of Physical Chemistry A, 2015, 119, 11623-11631.	2.5	81
4	Assessing Gaussian Process Regression and Permutationally Invariant Polynomial Approaches To Represent High-Dimensional Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2018, 14, 3381-3396.	5.3	78
5	Communication: VSCF/VCI vibrational spectroscopy of H7O3+ and H9O4+ using high-level, many-body potential energy surface and dipole moment surfaces. Journal of Chemical Physics, 2017, 146, 121102.	3.0	56
6	Development of nuclear basis sets for multicomponent quantum chemistry methods. Journal of Chemical Physics, 2020, 152, 244123.	3.0	47
7	Disentangling the Complex Vibrational Spectrum of the Protonated Water Trimer, H⁺(H₂O)₃, with Two-Color IR-IR Photodissociation of the Bare Ion and Anharmonic VSCF/VCI Theory. Journal of Physical Chemistry Letters, 2017, 8, 3782-3789.	4.6	44
8	High-Level Quantum Calculations of the IR Spectra of the Eigen, Zundel, and Ring Isomers of H⁺(H₂O)₄ Find a Single Match to Experiment. Journal of the American Chemical Society, 2017, 139, 10984-10987.	13.7	43
9	Communication: Spectroscopic consequences of proton delocalization in OCHCO+. Journal of Chemical Physics, 2015, 143, 071102.	3.0	42
10	q-AQUA: A Many-Body CCSD(T) Water Potential, Including Four-Body Interactions, Demonstrates the Quantum Nature of Water from Clusters to the Liquid Phase. Journal of Physical Chemistry Letters, 2022, 13, 5068-5074.	4.6	41
11	Benchmark Electronic Structure Calculations for H₃O⁺(H₂O)_n, n = 0â€“5, Clusters and Tests of an Existing 1,2,3-Body Potential Energy Surface with a New 4-Body Correction. Journal of Chemical Theory and Computation, 2018, 14, 4553-4566.	5.3	39
12	Deconstructing Prominent Bands in the Terahertz Spectra of H7O3+ and H9O4+: Intermolecular Modes in Eigen Clusters. Journal of Physical Chemistry Letters, 2018, 9, 798-803.	4.6	38
13	Classical, Thermostated Ring Polymer, and Quantum VSCF/VCI Calculations of IR Spectra of H₇O₃⁺ and H₉O₄⁺ (Eigen) and Comparison with Experiment. Journal of Physical Chemistry A, 2019, 123, 1399-1409.	2.5	34
14	Ab Initio Potential for H₃O⁺ â†' H⁺ + H₂O: A Step to a Many-Body Representation of the Hydrated Proton?. Journal of Chemical Theory and Computation, 2016, 12, 5284-5292.	5.3	30
15	Tag-Free and Isotopomer-Selective Vibrational Spectroscopy of the Cryogenically Cooled H₉O₄⁺ Cation with Two-Color, IRâ€“IR Double-Resonance Photoexcitation: Isolating the Spectral Signature of a Single OH Group in the Hydronium Ion Core. Journal of Physical Chemistry A, 2018, 122, 9275-9284.	2.5	27
16	A CCSD(T)-Based 4-Body Potential for Water. Journal of Physical Chemistry Letters, 2021, 12, 10318-10324.	4.6	25
17	Permutationally invariant polynomial regression for energies and gradients, using reverse differentiation, achieves orders of magnitude speed-up with high precision compared to other machine learning methods. Journal of Chemical Physics, 2022, 156, 044120.	3.0	24
18	High-Level VSCF/VCI Calculations Decode the Vibrational Spectrum of the Aqueous Proton. Journal of Physical Chemistry B, 2019, 123, 7214-7224.	2.6	23

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19	Tracking Hydronium/Water Stretches in Magic H₃O⁺(H₂O)₂₀ Clusters through High-level Quantum VSCF/VCI Calculations. Journal of Physical Chemistry A, 2020, 124, 1167-1175.	2.5	23
20	How the Zundel (H₅O₂⁺) Potential Can Be Used to Predict the Proton Stretch and Bend Frequencies of Larger Protonated Water Clusters. Journal of Physical Chemistry Letters, 2016, 7, 5259-5265.	4.6	20
21	Decoding the 2D IR spectrum of the aqueous proton with high-level VSCF/VCI calculations. Journal of Chemical Physics, 2020, 153, 124506.	3.0	20
22	Direct Dynamics with Nuclearâ€“Electronic Orbital Density Functional Theory. Accounts of Chemical Research, 2021, 54, 4131-4141.	15.6	19
23	Vibrational second-order perturbation theory (VPT2) using local monomer normal modes. Molecular Physics, 2015, 113, 3964-3971.	1.7	17
24	Disentangling the Complex Vibrational Mechanics of the Protonated Water Trimer by Rational Control of Its Hydrogen Bonds. Journal of Physical Chemistry A, 2019, 123, 7965-7972.	2.5	16
25	Nuclear-Electronic Orbital Multistate Density Functional Theory. Journal of Physical Chemistry Letters, 2020, 11, 10106-10113.	4.6	16
26	The MD17 datasets from the perspective of datasets for gas-phase â€œsmallâ€•molecule potentials. Journal of Chemical Physics, 2022, 156, .	3.0	12
27	Spectral analyses of trans- and cis-DOCO transients via comb spectroscopy. Molecular Physics, 2018, 116, 3710-3717.	1.7	7
28	Teaching vibrational spectra to assign themselves. Faraday Discussions, 2018, 212, 65-82.	3.2	3
29	Analytical gradients for nuclearâ€“electronic orbital multistate density functional theory: Geometry optimizations and reaction paths. Journal of Chemical Physics, 2022, 156, 114115.	3.0	2
30	MULTIMODE, The n-Mode Representation of the Potential and Illustrations to IR Spectra of Glycine and Two Protonated Water Clusters. , 2022, , 296-339.		1