Qi Yu

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/3367633/publications.pdf

Version: 2024-02-01

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 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
2	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
3	The MD17 datasets from the perspective of datasets for gas-phase â€œsmallâ€•molecule potentials. Journal of Chemical Physics, 2022, 156, .	3.0	12
4	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
5	MULTIMODE, The n-Mode Representation of the Potential and Illustrations to IR Spectra of Glycine and Two Protonated Water Clusters. , 2022, , 296-339.		1
6	Crossover from hydrogen to chemical bonding. Science, 2021, 371, 160-164.	12.6	123
7	A CCSD(T)-Based 4-Body Potential for Water. Journal of Physical Chemistry Letters, 2021, 12, 10318-10324.	4.6	25
8	Direct Dynamics with Nuclearâ€“Electronic Orbital Density Functional Theory. Accounts of Chemical Research, 2021, 54, 4131-4141.	15.6	19
9	Nuclear-Electronic Orbital Multistate Density Functional Theory. Journal of Physical Chemistry Letters, 2020, 11, 10106-10113.	4.6	16
10	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
11	Development of nuclear basis sets for multicomponent quantum chemistry methods. Journal of Chemical Physics, 2020, 152, 244123.	3.0	47
12	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
13	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
14	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
15	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
16	Permutationally Invariant Potential Energy Surfaces. Annual Review of Physical Chemistry, 2018, 69, 151-175.	10.8	152
17	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
18	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

#	Article	IF	Citations
19	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
20	Teaching vibrational spectra to assign themselves. Faraday Discussions, 2018, 212, 65-82.	3.2	3
21	Spectral analyses of trans- and cis-DOCO transients via comb spectroscopy. Molecular Physics, 2018, 116, 3710-3717.	1.7	7
22	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
23	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
24	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
25	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
26	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
27	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
28	Communication: Spectroscopic consequences of proton delocalization in OCHCO+. Journal of Chemical Physics, 2015, 143, 071102.	3.0	42
29	Structure, Anharmonic Vibrational Frequencies, and Intensities of NNHNN⁺. Journal of Physical Chemistry A, 2015, 119, 11623-11631.	2.5	81
30	Vibrational second-order perturbation theory (VPT2) using local monomer normal modes. Molecular Physics, 2015, 113, 3964-3971.	1.7	17