Chen Qu

List of Publications by Year
in descending order

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54	1,460	304602	330025
papers	citations	22 h-index	37 g-index

55	55	55	1239
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.	4.8	152
2	Two-Dimensional Morphology Enhances Light-Driven H₂ Generation Efficiency in CdS Nanoplatelet-Pt Heterostructures. Journal of the American Chemical Society, 2018, 140, 11726-11734.	6.6	106
3	Î” -machine learning for potential energy surfaces: A PIP approach to bring a DFT-based PES to CCSD(T) level of theory. Journal of Chemical Physics, 2021, 154, 051102.	1.2	89
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.	2.3	78
5	An ab initio potential energy surface for the formic acid dimer: zero-point energy, selected anharmonic fundamental energies, and ground-state tunneling splitting calculated in relaxed 1â€“4-mode subspaces. Physical Chemistry Chemical Physics, 2016, 18, 24835-24840.	1.3	76
6	Capturing roaming molecular fragments in real time. Science, 2020, 370, 1072-1077.	6.0	61
7	Permutationally Invariant Fitting of Many-Body, Non-covalent Interactions with Application to Three-Body Methaneâ€“Waterâ€“Water. Journal of Chemical Theory and Computation, 2015, 11, 1631-1638.	2.3	60
8	â€œPlug and playâ€•full-dimensional ab initio potential energy and dipole moment surfaces and anharmonic vibrational analysis for CH₄â€“H₂O. Physical Chemistry Chemical Physics, 2015, 17, 8172-8181.	1.3	54
9	Using Gradients in Permutationally Invariant Polynomial Potential Fitting: A Demonstration for CH₄ Using as Few as 100 Configurations. Journal of Chemical Theory and Computation, 2019, 15, 2826-2835.	2.3	43
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.	2.1	41
11	Full-dimensional, high-level ab initio potential energy surfaces for H2(H2O) and H2(H2O)2 with application to hydrogen clathrate hydrates. Journal of Chemical Physics, 2015, 143, 084302.	1.2	40
12	Breaking the Coupled Cluster Barrier for Machine-Learned Potentials of Large Molecules: The Case of 15-Atom Acetylacetone. Journal of Physical Chemistry Letters, 2021, 12, 4902-4909.	2.1	39
13	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.	2.1	38
14	A fragmented, permutationally invariant polynomial approach for potential energy surfaces of large molecules: Application to N-methyl acetamide. Journal of Chemical Physics, 2019, 150, 141101.	1.2	37
15	Quantum approaches to vibrational dynamics and spectroscopy: is ease of interpretation sacrificed as rigor increases?. Physical Chemistry Chemical Physics, 2019, 21, 3397-3413.	1.3	35
16	Efficient Generation of Permutationally Invariant Potential Energy Surfaces for Large Molecules. Journal of Chemical Theory and Computation, 2020, 16, 3264-3272.	2.3	33
17	Full and fragmented permutationally invariant polynomial potential energy surfaces for trans and cis N-methyl acetamide and isomerization saddle points. Journal of Chemical Physics, 2019, 151, 084306.	1.2	32
18	Revisiting Adiabatic Switching for Initial Conditions in Quasi-Classical Trajectory Calculations: Application to CH₄. Journal of Physical Chemistry A, 2016, 120, 4988-4993.	1.1	30

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19	Permutationally invariant polynomial potential energy surfaces for tropolone and H and D atom tunneling dynamics. Journal of Chemical Physics, 2020, 153, 024107.	1.2	27
20	Full-Dimensional Quantum Dynamics of SiO in Collision with H₂. Journal of Physical Chemistry A, 2018, 122, 1511-1520.	1.1	25
21	Observation of the Lowâ€Frequency Spectrum of the Water Dimer as a Sensitive Test of the Water Dimer Potential and Dipole Moment Surfaces. Angewandte Chemie - International Edition, 2019, 58, 13119-13126.	7.2	25
22	A CCSD(T)-Based 4-Body Potential for Water. Journal of Physical Chemistry Letters, 2021, 12, 10318-10324.	2.1	25
23	Full-dimensional potential energy surface for acetylacetone and tunneling splittings. Physical Chemistry Chemical Physics, 2021, 23, 7758-7767.	1.3	24
24	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.	1.2	24
25	High-dimensional fitting of sparse datasets of CCSD(T) electronic energies and MP2 dipole moments, illustrated for the formic acid dimer and its complex IR spectrum. Journal of Chemical Physics, 2018, 148, 241713.	1.2	23
26	Full-dimensional, ab initio potential energy surface for glycine with characterization of stationary points and zero-point energy calculations by means of diffusion Monte Carlo and semiclassical dynamics. Journal of Chemical Physics, 2020, 153, 244301.	1.2	23
27	IR Spectra of (HCOOH)₂ and (DCOOH)₂: Experiment, VSCF/VCI, and Ab Initio Molecular Dynamics Calculations Using Full-Dimensional Potential and Dipole Moment Surfaces. Journal of Physical Chemistry Letters, 2018, 9, 2604-2610.	2.1	22
28	Predicting KovÃ¡ts Retention Indices Using Graph Neural Networks. Journal of Chromatography A, 2021, 1646, 462100.	1.8	18
29	Quantum and classical IR spectra of (HCOOH)₂, (DCOOH)₂ and (DCOOD)₂ using ab initio potential energy and dipole moment surfaces. Faraday Discussions, 2018, 212, 33-49.	1.6	17
30	Ab Initio, Embedded Local-Monomer Calculations of Methane Vibrational Energies in Clathrate Hydrates. Journal of Physical Chemistry C, 2016, 120, 3167-3175.	1.5	16
31	Observation of the Lowâ€Frequency Spectrum of the Water Trimer as a Sensitive Test of the Waterâ€Trimer Potential and the Dipoleâ€Moment Surface. Angewandte Chemie - International Edition, 2020, 59, 11399-11407.	7.2	16
32	MULTIMODE calculations of the infrared spectra of H 7 + and D 7 + using ab initio potential energy and dipole moment surfaces. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	14
33	The MD17 datasets from the perspective of datasets for gas-phase â€œsmallâ€•molecule potentials. Journal of Chemical Physics, 2022, 156, .	1.2	12
34	Assessing the Importance of the H₂â€“H₂Oâ€“H₂O Three-Body Interaction on the Vibrational Frequency Shift of H₂ in the sII Clathrate Hydrate and Comparison with Experiment. Journal of Physical Chemistry A, 2019, 123, 329-335.	1.1	11
35	Full-dimensional, ab initio potential energy surface for CH₃OHâ€‰â†’â€‰CH₃+OH. Molecular Physics, 2013, 111, 1964-1971.	0.8	10
36	Full-dimensional quantum dynamics of SO(X<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 82 Td (xmlns:mml="http://www.w3.org/1 in collision with H2. Chemical Physics, 2020, 532, 110695.	0.9	10

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37	Full-dimensional quantum calculations of the dissociation energy, zero-point, and 10 K properties of ${m H}_{7}^{+}$H7+/${m D}_{7}^{+}$D7+ clusters using an ab initio potential energy surface. Journal of Chemical Physics, 2013, 139, 024308.	1.2	9
38	Inelastic vibrational dynamics of CS in collision with H₂ using a full-dimensional potential energy surface. Physical Chemistry Chemical Physics, 2018, 20, 28425-28434.	1.3	9
39	MULTIMODE Calculations of Vibrational Spectroscopy and 1d Interconformer Tunneling Dynamics in Glycine Using a Full-Dimensional Potential Energy Surface. Journal of Physical Chemistry A, 2021, 125, 5346-5354.	1.1	9
40	Graph convolutional neural network applied to the prediction of normal boiling point. Journal of Molecular Graphics and Modelling, 2022, 112, 108149.	1.3	9
41	A molecular road movie. Physics Today, 2021, 74, 62-63.	0.3	7
42	Observation of the Lowâ€Frequency Spectrum of the Water Dimer as a Sensitive Test of the Water Dimer Potential and Dipole Moment Surfaces. Angewandte Chemie, 2019, 131, 13253-13260.	1.6	5
43	Diffusion Monte Carlo with fictitious masses finds holes in potential energy surfaces. Molecular Physics, 0, , .	0.8	5
44	Electronic relaxation and dissociation dynamics in formaldehyde: pump wavelength dependence. Physical Chemistry Chemical Physics, 2022, 24, 1779-1786.	1.3	5
45	Does Infrared Multiphoton Dissociation of Vinyl Chloride Yield Cold Vinylidene?. Journal of Physical Chemistry Letters, 2015, 6, 2457-2462.	2.1	4
46	Diffusion Monte Carlo Calculations of Zero-Point Structures of Partially Deuterated Isotopologues of H₇⁺. Journal of Physical Chemistry B, 2014, 118, 8221-8226.	1.2	3
47	Teaching vibrational spectra to assign themselves. Faraday Discussions, 2018, 212, 65-82.	1.6	3
48	Diffusion Monte Carlo Calculations of Zeroâ€Point Energies of Methanol and Deuterated Methanol. Journal of Computational Chemistry, 2019, 40, 328-332.	1.5	3
49	MULTIMODE, The n-Mode Representation of the Potential and Illustrations to IR Spectra of Glycine and Two Protonated Water Clusters. , 2022, , 296-339.		1
50	Frontispiz: Observation of the Lowâ€Frequency Spectrum of the Water Trimer as a Sensitive Test of the Waterâ€Trimer Potential and the Dipoleâ€Moment Surface. Angewandte Chemie, 2020, 132, .	1.6	0
51	Observation of the Lowâ€Frequency Spectrum of the Water Trimer as a Sensitive Test of the Waterâ€Trimer Potential and the Dipoleâ€Moment Surface. Angewandte Chemie, 2020, 132, 11496-11504.	1.6	0
52	Frontispiece: Observation of the Lowâ€Frequency Spectrum of the Water Trimer as a Sensitive Test of the Waterâ€Trimer Potential and the Dipoleâ€Moment Surface. Angewandte Chemie - International Edition, 2020, 59, .	7.2	0
53	On the measurement of statistical dynamics using the method of Coulomb explosion imaging. AIP Conference Proceedings, 2021, , .	0.3	0
54	Capturing Roaming Fragments in Real Time: A Molecular Road Movie. , 2020, , .		0