Chen Qu

List of Publications by Year in Descending Order

49 papers	898 citations	17 h-index	28 g-index
55 ext. papers	1,178 ext. citations	5.6 avg, IF	5.22 L-index

#	Paper	IF	Citations
49	Graph convolutional neural network applied to the prediction of normal boiling point.. *Journal of Molecular Graphics and Modelling*, **2022**, 112, 108149	2.8	1
48	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	3.9	4
47	MULTIMODE, The n-Mode Representation of the Potential and Illustrations to IR Spectra of Glycine and Two Protonated Water Clusters **2022**, 296-339		1
46	A CCSD(T)-Based 4-Body Potential for Water. *Journal of Physical Chemistry Letters*, **2021**, 12, 10318-10324	6.4	3
45	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	6.4	13
44	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	2.8	1
43	Predicting Kovᵻs Retention Indices Using Graph Neural Networks. *Journal of Chromatography A*, **2021**, 1646, 462100	4.5	5
42	A molecular road movie. *Physics Today*, **2021**, 74, 62-63	0.9	1
41	Full-dimensional potential energy surface for acetylacetone and tunneling splittings. *Physical Chemistry Chemical Physics*, **2021**, 23, 7758-7767	3.6	14
40	ᵻmachine 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	3.9	34
39	Observation of the Low-Frequency Spectrum of the Water Trimer as a Sensitive Test of the Water-Trimer Potential and the Dipole-Moment Surface. *Angewandte Chemie*, **2020**, 132, 11496-11504	3.6	
38	Efficient Generation of Permutationally Invariant Potential Energy Surfaces for Large Molecules. *Journal of Chemical Theory and Computation*, **2020**, 16, 3264-3272	6.4	21
37	Permutationally invariant polynomial potential energy surfaces for tropolone and H and D atom tunneling dynamics. *Journal of Chemical Physics*, **2020**, 153, 024107	3.9	12
36	Full-dimensional quantum dynamics of SO(X3ᵻ) in collision with H2. *Chemical Physics*, **2020**, 532, 110695	2.3	4
35	Observation of the Low-Frequency Spectrum of the Water Trimer as a Sensitive Test of the Water-Trimer Potential and the Dipole-Moment Surface. *Angewandte Chemie - International Edition*, **2020**, 59, 11399-11407	16.4	4
34	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	3.9	11
33	Capturing roaming molecular fragments in real time. *Science*, **2020**, 370, 1072-1077	33.3	22

32	Quantum approaches to vibrational dynamics and spectroscopy: is ease of interpretation sacrificed as rigor increases?. *Physical Chemistry Chemical Physics*, **2019**, 21, 3397-3413	3.6	27
31	Using Gradients in Permutationally Invariant Polynomial Potential Fitting: A Demonstration for CH Using as Few as 100 Configurations. *Journal of Chemical Theory and Computation*, **2019**, 15, 2826-2835	6.4	25
30	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	3.9	26
29	Observation of the Low-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	3.6	4
28	Observation of the Low-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	16.4	19
27	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	3.9	24
26	Assessing the Importance of the H-HO-HO Three-Body Interaction on the Vibrational Frequency Shift of H in the sII Clathrate Hydrate and Comparison with Experiment. *Journal of Physical Chemistry A*, **2019**, 123, 329-335	2.8	5
25	Diffusion Monte Carlo Calculations of Zero-Point Energies of Methanol and Deuterated Methanol. *Journal of Computational Chemistry*, **2019**, 40, 328-332	3.5	3
24	Permutationally Invariant Potential Energy Surfaces. *Annual Review of Physical Chemistry*, **2018**, 69, 151-175	13.7	107
23	Full-Dimensional Quantum Dynamics of SiO in Collision with H. *Journal of Physical Chemistry A*, **2018**, 122, 1511-1520	2.8	16
22	Deconstructing Prominent Bands in the Terahertz Spectra of HO and HO: Intermolecular Modes in Eigen Clusters. *Journal of Physical Chemistry Letters*, **2018**, 9, 798-803	6.4	27
21	Quantum and classical IR spectra of (HCOOH), (DCOOH) and (DCOOD) using ab initio potential energy and dipole moment surfaces. *Faraday Discussions*, **2018**, 212, 33-49	3.6	13
20	IR Spectra of (HCOOH) and (DCOOH): 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	6.4	15
19	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	3.9	16
18	Adiabatic Switching Applied to the Vibrations of syn-CH3CHOO and Implications for Zero-Point Leak and Isomerization in Quasiclassical Trajectory Calculations. *Advances in Chemical Physics*, **2018**, 151-166		1
17	Two-Dimensional Morphology Enhances Light-Driven H Generation Efficiency in CdS Nanoplatelet-Pt Heterostructures. *Journal of the American Chemical Society*, **2018**, 140, 11726-11734	16.4	87
16	Inelastic vibrational dynamics of CS in collision with H using a full-dimensional potential energy surface. *Physical Chemistry Chemical Physics*, **2018**, 20, 28425-28434	3.6	6
15	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	6.4	57

14	Teaching vibrational spectra to assign themselves. *Faraday Discussions*, **2018**, 212, 65-82	3.6	3
13	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 1-4-mode subspaces. *Physical Chemistry Chemical Physics*, **2016**, 18, 24835-24840	3.6	53
12	Revisiting Adiabatic Switching for Initial Conditions in Quasi-Classical Trajectory Calculations: Application to CH4. *Journal of Physical Chemistry A*, **2016**, 120, 4988-93	2.8	25
11	Ab Initio, Embedded Local-Monomer Calculations of Methane Vibrational Energies in Clathrate Hydrates. *Journal of Physical Chemistry C*, **2016**, 120, 3167-3175	3.8	16
10	Does Infrared Multiphoton Dissociation of Vinyl Chloride Yield Cold Vinylidene?. *Journal of Physical Chemistry Letters*, **2015**, 6, 2457-62	6.4	4
9	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	3.9	29
8	"Plug and play" full-dimensional ab initio potential energy and dipole moment surfaces and anharmonic vibrational analysis for CH4-H2O. *Physical Chemistry Chemical Physics*, **2015**, 17, 8172-81	3.6	47
7	Permutationally Invariant Fitting of Many-Body, Non-covalent Interactions with Application to Three-Body Methane-Water-Water. *Journal of Chemical Theory and Computation*, **2015**, 11, 1631-8	6.4	54
6	Diffusion Monte Carlo calculations of zero-point structures of partially deuterated isotopologues of H7(+). *Journal of Physical Chemistry B*, **2014**, 118, 8221-6	3.4	3
5	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	1.9	11
4	Full-dimensional, ab initio potential energy surface for CH3OH -¢CH3+OH. *Molecular Physics*, **2013**, 111, 1964-1971	1.7	8
3	Full-dimensional quantum calculations of the dissociation energy, zero-point, and 10 K properties of H7+/D7+ clusters using an ab initio potential energy surface. *Journal of Chemical Physics*, **2013**, 139, 024308	3.9	9
2	Diffusion Monte Carlo with fictitious masses finds holes in potential energy surfaces. *Molecular Physics*,	1.7	1
1	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*,5068-5074	6.4	6