Paul L Houston

List of Publications by Year in Descending Order

53 papers	2,324 citations	23 h-index	48 g-index
57 ext. papers	2,607 ext. citations	5.9 avg, IF	5.16 L-index

#	Paper	IF	Citations
53	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
52	MULTIMODE, The n-Mode Representation of the Potential and Illustrations to IR Spectra of Glycine and Two Protonated Water Clusters **2022**, 296-339		1
51	A CCSD(T)-Based 4-Body Potential for Water. *Journal of Physical Chemistry Letters*, **2021**, 12, 10318-10324	6.4	3
50	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
49	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
48	Full-dimensional potential energy surface for acetylacetone and tunneling splittings. *Physical Chemistry Chemical Physics*, **2021**, 23, 7758-7767	3.6	14
47	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	3.9	34
46	A Machine Learning Approach for Rate Constants. II. Clustering, Training, and Predictions for the O(P) + HCl -> OH + Cl Reaction. *Journal of Physical Chemistry A*, **2020**, 124, 5746-5755	2.8	16
45	Efficient Generation of Permutationally Invariant Potential Energy Surfaces for Large Molecules. *Journal of Chemical Theory and Computation*, **2020**, 16, 3264-3272	6.4	21
44	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
43	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
42	Capturing roaming molecular fragments in real time. *Science*, **2020**, 370, 1072-1077	33.3	22
41	Rotational resonances in the HCO roaming reaction are revealed by detailed correlations. *Science*, **2020**, 369, 1592-1596	33.3	16
40	A Tribute to William M. Jackson, Jr. *Journal of Physical Chemistry A*, **2019**, 123, 1905-1907	2.8	
39	A Machine Learning Approach for Prediction of Rate Constants. *Journal of Physical Chemistry Letters*, **2019**, 10, 5250-5258	6.4	15
38	H atom Product Channels in the Ultraviolet Photodissociation of the 2-Propenyl Radical. *Journal of Physical Chemistry A*, **2019**, 123, 9957-9965	2.8	5
37	Teaching vibrational spectra to assign themselves. *Faraday Discussions*, **2018**, 212, 65-82	3.6	3

36	Formaldehyde roaming dynamics: Comparison of quasi-classical trajectory calculations and experiments. *Journal of Chemical Physics*, **2017**, 147, 013936	3.9	16
35	Perspective: Advanced particle imaging. *Journal of Chemical Physics*, **2017**, 147, 013601	3.9	32
34	A new (multi-reference configuration interaction) potential energy surface for HCO and preliminary studies of roaming. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2017**, 375,	3	29
33	Theories and simulations of roaming. *Chemical Society Reviews*, **2017**, 46, 7615-7624	58.5	51
32	Roaming Under the Microscope: Trajectory Study of Formaldehyde Dissociation. *Journal of Physical Chemistry A*, **2016**, 120, 5103-14	2.8	38
31	Ultraviolet Photodissociation Dynamics of the 1-Propenyl Radical. *Journal of Physical Chemistry A*, **2016**, 120, 5248-56	2.8	8
30	Trajectory and Model Studies of Collisions of Highly Excited Methane with Water Using an ab Initio Potential. *Journal of Physical Chemistry A*, **2015**, 119, 12304-17	2.8	17
29	"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
28	A model for energy transfer in collisions of atoms with highly excited molecules. *Journal of Physical Chemistry A*, **2015**, 119, 4695-710	2.8	11
27	Collisional energy transfer in highly excited molecules. *Journal of Physical Chemistry A*, **2014**, 118, 7758-75	2.8	17
26	Two roaming pathways in the photolysis of CH3CHO between 328 and 308 nm. *Chemical Science*, **2014**, 5, 4633-4638	9.4	43
25	Communication: A benchmark-quality, full-dimensional ab initio potential energy surface for Ar-HOCO. *Journal of Chemical Physics*, **2014**, 140, 151101	3.9	33
24	Classical trajectory study of energy transfer in collisions of highly excited allyl radical with argon. *Journal of Physical Chemistry A*, **2013**, 117, 14028-41	2.8	27
23	The dynamics of allyl radical dissociation. *Journal of Physical Chemistry A*, **2011**, 115, 6797-804	2.8	18
22	Evidence for Vinylidene Production in the Photodissociation of the Allyl Radical. *Journal of Physical Chemistry Letters*, **2010**, 1, 1875-1880	6.4	38
21	Electronic to Vibrational Energy Transfer from Excited Halogen Atoms. *Advances in Chemical Physics* , **2007**, 381-418		9
20	Initiation of Atom-Molecule Reactions by Infrared Multiphoton Dissociation. *Advances in Chemical Physics*, **2007**, 625-638		7
19	PHOTODISSOCIATION DYNAMICS OF OZONE IN THE HARTLEY BAND. *Advanced Series in Physical Chemistry*, **2004**, 281-327		6

18	Product Imaging Studies of Photodissociation and Bimolecular Reaction Dynamics. *Journal of the Chinese Chemical Society*, **2001**, 48, 309-318	1.5	5
17	The energy distribution, angular distribution, and alignment of the O(1D2) fragment from the photodissociation of ozone between 235 and 305 nm. *Journal of Chemical Physics*, **2001**, 115, 7460-7473	3.9	62
16	Evidence of a Double Surface Crossing between Open- and Closed-Shell Surfaces in the Photodissociation of Cyclopropyl Iodide. *Journal of Physical Chemistry A*, **2001**, 105, 1693-1701	2.8	23
15	Differential Cross Section for Rotationally Inelastic Scattering of Vibrationally Excited NO(v=5) from Ar. *Journal of Physical Chemistry A*, **2001**, 105, 11165-11170	2.8	16
14	The vibrational distribution of O2(X 3Σg−) produced in the photodissociation of ozone between 226 and 240 and at 266 nm. *Journal of Chemical Physics*, **2000**, 112, 1279-1286	3.9	48
13	Improvements in the Product Imaging Technique and Their Application to Ozone Photodissociation. *ACS Symposium Series*, **2000**, 34-55	0.4	
12	Changes in the Vibrational Population of SO(3Σ−) from the Photodissociation of SO2between 202 and 207 nm *Journal of Physical Chemistry A*, **2000**, 104, 10240-10246	2.8	24
11	Determination of the heat of formation of O3 using vacuum ultraviolet laser-induced fluorescence spectroscopy and two-dimensional product imaging techniques. *Journal of Chemical Physics*, **1999**, 111, 6350-6355	3.9	47
10	Zero Kinetic Energy Photofragment Spectroscopy: The Threshold Dissociation of NO2. *Journal of Physical Chemistry A*, **1998**, 102, 9666-9673	2.8	15
9	Improved two-dimensional product imaging: The real-time ion-counting method. *Review of Scientific Instruments*, **1998**, 69, 1665-1670	1.7	165
8	Speed-Dependent Anisotropy Parameters in the UV Photodissociation of Ozone. *Journal of Physical Chemistry A*, **1997**, 101, 7593-7599	2.8	44
7	New Laser-Based and Imaging Methods for Studying the Dynamics of Molecular Collisions. *The Journal of Physical Chemistry*, **1996**, 100, 12757-12770		70
6	Photodissociation dynamics of state-selected resonances of HCO X 2A prepared by stimulated emission pumping. *Journal of Chemical Physics*, **1995**, 102, 1645-1657	3.9	48
5	Photodissociation dynamics of acetone at 193 nm: Photofragment internal and translational energy distributions. *Journal of Chemical Physics*, **1989**, 91, 7498-7513	3.9	129
4	Two-dimensional imaging of state-selected photodissociation products detected by multiphoton ionization. *Journal of Chemical Physics*, **1987**, 87, 1445-1447	3.9	809
3	Product correlations in photofragment dynamics. *Faraday Discussions of the Chemical Society*, **1986**, 82, 13		40
2	Formaldehyde photochemistry: Appearance rate, vibrational relaxation, and energy distribution of the CO product. *Journal of Chemical Physics*, **1976**, 65, 757-770	3.9	135
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