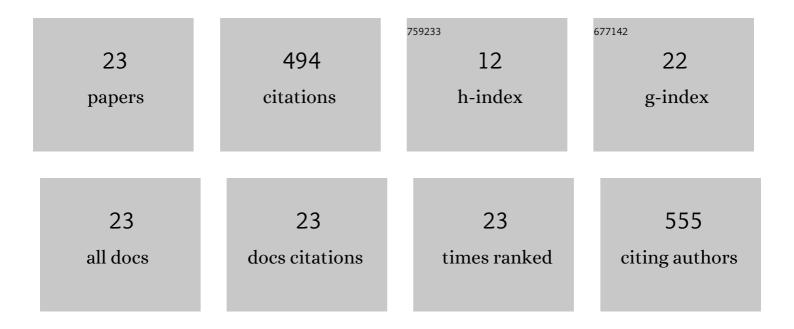


## List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Direct Chemical Dynamics Simulations. Journal of the American Chemical Society, 2017, 139, 3570-3590.	13.7	128
2	Perspective: chemical dynamics simulations of non-statistical reaction dynamics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20160204.	3.4	63
3	Advanced Materials for Energy-Water Systems: The Central Role of Water/Solid Interfaces in Adsorption, Reactivity, and Transport. Chemical Reviews, 2021, 121, 9450-9501.	47.7	43
4	Structural Characterization of Protonated Water Clusters Confined in HZSM-5 Zeolites. Journal of the American Chemical Society, 2021, 143, 10203-10213.	13.7	35
5	Potential energy surface stationary points and dynamics of the F <sup>â^'</sup> + CH <sub>3</sub> I double inversion mechanism. Physical Chemistry Chemical Physics, 2017, 19, 20127-20136.	2.8	31
6	Competing E2 and S <sub>N</sub> 2 Mechanisms for the F <sup>–</sup> + CH <sub>3</sub> CH <sub>2</sub> I Reaction. Journal of Physical Chemistry A, 2017, 121, 1078-1085.	2.5	26
7	Chemical Dynamics Simulations of Benzene Dimer Dissociation. Journal of Physical Chemistry A, 2015, 119, 6631-6640.	2.5	25
8	Effect of microsolvation on the OHâ^'(H2O)n+ CH3I rate constant. comparison of experiment and calculations for OHâ^'(H2O)2+ CH3I. International Journal of Mass Spectrometry, 2017, 418, 122-129.	1.5	20
9	A quantum mechanical insight into SN2 reactions: Semiclassical initial value representation calculations of vibrational features of the Clâ^âcCH3Cl pre-reaction complex with the VENUS suite of codes. Journal of Chemical Physics, 2018, 149, 164113.	3.0	19
10	Post-transition state dynamics and product energy partitioning following thermal excitation of the Fâ‹-HCH2CN transition state: Disagreement with experiment. Journal of Chemical Physics, 2017, 147, 144301.	3.0	14
11	Model-Based Analyses of Confined Polymer Electrolyte Nanothin Films Experimentally Probed by Polarized ATR–FTIR Spectroscopy. Journal of Physical Chemistry C, 2018, 122, 9578-9585.	3.1	13
12	Direct dynamics simulations of the unimolecular dissociation of dioxetane: Probing the non-RRKM dynamics. Journal of Chemical Physics, 2018, 148, 164309.	3.0	12
13	Water-Assisted Proton Transport in Confined Nanochannels. Journal of Physical Chemistry C, 2020, 124, 16186-16201.	3.1	12
14	Effects of vibrational and rotational energies on the lifetime of the pre-reaction complex for the Fâ^'+ CH3I SN2 reaction. International Journal of Mass Spectrometry, 2018, 429, 127-135.	1.5	11
15	Anharmonic Densities of States for Vibrationally Excited I <sup>–</sup> (H <sub>2</sub> O), (H <sub>2</sub> O) <sub>2</sub> , and I <sup>–</sup> (H <sub>2</sub> O) <sub>2</sub> . Journal of Chemical Theory and Computation, 2018, 14, 3986-3997.	5.3	8
16	Single Solvent Molecules Induce Dual Nucleophiles in Gas-Phase Ion–Molecule Nucleophilic Substitution Reactions. Journal of Physical Chemistry Letters, 2021, 12, 7134-7139.	4.6	8
17	PSO Method for Fitting Analytic Potential Energy Functions. Application to I–(H2O). Journal of Chemical Theory and Computation, 2018, 14, 1321-1332.	5.3	5
18	Interaction between γC87 and γR242 residues participates in energy coupling between catalysis and proton translocation in Escherichia coli ATP synthase. Biochimica Et Biophysica Acta - Bioenergetics, 2019, 1860, 679-687.	1.0	5

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19	Pronounced changes in atomistic mechanisms for the Cl <sup>â^²</sup> + CH <sub>3</sub> 1 S <sub>N</sub> 2 reaction with increasing collision energy. Physical Chemistry Chemical Physics, 2019, 21, 2039-2045.	2.8	5
20	ls CH3NC isomerization an intrinsic non-RRKM unimolecular reaction?. Journal of Chemical Physics, 2019, 151, 184110.	3.0	4
21	Addressing an instability in unrestricted density functional theory direct dynamics simulations. Journal of Computational Chemistry, 2019, 40, 933-936.	3.3	3
22	Differential Condensation of Methane Isotopologues Leading to Isotopic Enrichment under Non-equilibrium Gas–Surface Collision Conditions. Journal of Physical Chemistry A, 2021, 125, 9405-9413.	2.5	3
23	Time-Dependent Perspective for the Intramolecular Couplings of the N–H Stretches of Protonated Tryptophan. Journal of Physical Chemistry A, 2020, 124, 4062-4067.	2.5	1