Baron Peters

List of Publications by Citations

102 papers	6,497 citations	37 h-index	80 g-index
110 ext. papers	7,307 ext. citations	6.8 avg, IF	6.09 L-index

#	Paper	IF	Citations
102	Advances in methods and algorithms in a modern quantum chemistry program package. *Physical Chemistry Chemical Physics*, **2006**, 8, 3172-91	3.6	2371
101	Obtaining reaction coordinates by likelihood maximization. *Journal of Chemical Physics*, **2006**, 125, 054108	3.9	265
100	A growing string method for determining transition states: comparison to the nudged elastic band and string methods. *Journal of Chemical Physics*, **2004**, 120, 7877-86	3.9	257
99	Homogeneous nucleation of methane hydrates: unrealistic under realistic conditions. *Journal of the American Chemical Society*, **2012**, 134, 19544-7	16.4	188
98	Strictosidine synthase: mechanism of a Pictet-Spengler catalyzing enzyme. *Journal of the American Chemical Society*, **2008**, 130, 710-23	16.4	162
97	Molecular-level origins of biomass recalcitrance: decrystallization free energies for four common cellulose polymorphs. *Journal of Physical Chemistry B*, **2011**, 115, 4118-27	3.4	161
96	Comprehensive DFT study of nitrous oxide decomposition over Fe-ZSM-5. *Journal of Physical Chemistry B*, **2005**, 109, 1857-73	3.4	156
95	Extensions to the likelihood maximization approach for finding reaction coordinates. *Journal of Chemical Physics*, **2007**, 127, 034109	3.9	139
94	Role of stacking disorder in ice nucleation. *Nature*, **2017**, 551, 218-222	50.4	132
93	Nucleation of NaCl from Aqueous Solution: Critical Sizes, Ion-Attachment Kinetics, and Rates. *Journal of the American Chemical Society*, **2015**, 137, 13352-61	16.4	116
92	Path sampling calculation of methane diffusivity in natural gas hydrates from a water-vacancy assisted mechanism. *Journal of the American Chemical Society*, **2008**, 130, 17342-50	16.4	113
91	Polyethylene upcycling to long-chain alkylaromatics by tandem hydrogenolysis/aromatization. *Science*, **2020**, 370, 437-441	33.3	110
90	Reaction Coordinates and Mechanistic Hypothesis Tests. *Annual Review of Physical Chemistry*, **2016**, 67, 669-90	15.7	95
89	Transmission Coefficients, Committors, and Solvent Coordinates in Ion-Pair Dissociation. *Journal of Chemical Theory and Computation*, **2014**, 10, 659-67	6.4	89
88	Beyond Ordered Materials: Understanding Catalytic Sites on Amorphous Solids. *ACS Catalysis*, **2017**, 7, 7543-7557	13.1	84
87	Catalytic upcycling of high-density polyethylene via a processive mechanism. *Nature Catalysis*, **2020**, 3, 893-901	36.5	78
86	Surface-mediated nucleation in the solid-state polymorph transformation of terephthalic acid. *Journal of the American Chemical Society*, **2007**, 129, 4714-23	16.4	76

85	Methane Clathrate Hydrate Nucleation Mechanism by Advanced Molecular Simulations. *Journal of Physical Chemistry C*, **2014**, 118, 22847-22857	3.8	72
84	Using the histogram test to quantify reaction coordinate error. *Journal of Chemical Physics*, **2006**, 125, 241101	3.9	69
83	Asparagine deamidation: pH-dependent mechanism from density functional theory. *Biochemistry*, **2006**, 45, 5384-92	3.2	68
82	Computational Kinetic Discrimination of Ethylene Polymerization Mechanisms for the Phillips (Cr/SiO2) Catalyst. *ACS Catalysis*, **2015**, 5, 3360-3374	13.1	63
81	Competing nucleation pathways in a mixture of oppositely charged colloids: out-of-equilibrium nucleation revisited. *Journal of Chemical Physics*, **2009**, 131, 244103	3.9	60
80	Reaction coordinates, one-dimensional Smoluchowski equations, and a test for dynamical self-consistency. *Journal of Chemical Physics*, **2013**, 138, 054106	3.9	58
79	Size-Dependent Surface Free Energy and Tolman-Corrected Droplet Nucleation of TIP4P/2005 Water. *Journal of Physical Chemistry Letters*, **2013**, 4, 4267-72	6.4	54
78	Synthesis and characterization of a Cu14 hydride cluster supported by neutral donor ligands. *Chemistry - A European Journal*, **2015**, 21, 5341-4	4.8	50
77	Pre-ordering of interfacial water in the pathway of heterogeneous ice nucleation does not lead to a two-step crystallization mechanism. *Journal of Chemical Physics*, **2016**, 145, 211910	3.9	49
76	Optimizing Nucleus Size Metrics for Liquid-Solid Nucleation from Transition Paths of Near-Nanosecond Duration. *Journal of Physical Chemistry Letters*, **2011**, 2, 1133-8	6.4	48
75	Nucleation in a Potts lattice gas model of crystallization from solution. *Journal of Chemical Physics*, **2009**, 131, 184101	3.9	47
74	Recent advances in transition path sampling: accurate reaction coordinates, likelihood maximisation and diffusive barrier-crossing dynamics. *Molecular Simulation*, **2010**, 36, 1265-1281	2	46
73	Communication: Bubbles, crystals, and laser-induced nucleation. *Journal of Chemical Physics*, **2011**, 134, 171102	3.9	45
72	NaCl nucleation from brine in seeded simulations: Sources of uncertainty in rate estimates. *Journal of Chemical Physics*, **2018**, 148, 222838	3.9	45
71	Inertial likelihood maximization for reaction coordinates with high transmission coefficients. *Chemical Physics Letters*, **2012**, 554, 248-253	2.5	44
70	Evidence for a size dependent nucleation mechanism in solid state polymorph transformations. *Journal of Physical Chemistry B*, **2008**, 112, 7460-6	3.4	44
69	Communication: an existence test for dividing surfaces without recrossing. *Journal of Chemical Physics*, **2014**, 140, 041104	3.9	43
68	One-Electron-Redox Activation of the Reduced Phillips Polymerization Catalyst, via Alkylchromium(IV) Homolysis: A Computational Assessment. *ACS Catalysis*, **2016**, 6, 6073-6085	13.1	42

67	Nucleation and Growth Kinetics from LaMer Burst Data. *Journal of Physical Chemistry A*, **2017**, 121, 7511-7517	2.8	42
66	Common features of extraordinary rate theories. *Journal of Physical Chemistry B*, **2015**, 119, 6349-56	3.4	40
65	Ion dissolution mechanism and kinetics at kink sites on NaCl surfaces. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 656-661	11.5	37
64	Supersaturation rates and schedules: Nucleation kinetics from isothermal metastable zone widths. *Journal of Crystal Growth*, **2011**, 317, 79-83	1.6	33
63	A Stochastic Model for Nucleation in the Boundary Layer during Solvent Freeze-Concentration. *Crystal Growth and Design*, **2013**, 13, 4642-4647	3.5	32
62	Rate-Enhancing Roles of Water Molecules in Methyltrioxorhenium-Catalyzed Olefin Epoxidation by Hydrogen Peroxide. *Journal of the American Chemical Society*, **2015**, 137, 9604-16	16.4	31
61	Single atom catalysts on amorphous supports: A quenched disorder perspective. *Journal of Chemical Physics*, **2015**, 142, 104708	3.9	31
60	Isolated catalyst sites on amorphous supports: a systematic algorithm for understanding heterogeneities in structure and reactivity. *Journal of Chemical Physics*, **2013**, 138, 204105	3.9	30
59	The Clathrate-Water Interface Is Oleophilic. *Journal of Physical Chemistry Letters*, **2018**, 9, 3224-3231	6.4	30
58	Ligand Exchange-Mediated Activation and Stabilization of a Re-Based Olefin Metathesis Catalyst by Chlorinated Alumina. *Journal of the American Chemical Society*, **2016**, 138, 12935-12947	16.4	29
57	A simulation test of the optical Kerr mechanism for laser-induced nucleation. *Journal of Chemical Physics*, **2011**, 134, 154501	3.9	29
56	Solute Precipitate Nucleation: A Review of Theory and Simulation Advances. *Advances in Chemical Physics*, **2014**, 97-160		28
55	Rate Expressions for Kink Attachment and Detachment During Crystal Growth. *Crystal Growth and Design*, **2016**, 16, 3313-3322	3.5	28
54	Easy transition path sampling methods: flexible-length aimless shooting and permutation shooting. *Journal of Chemical Theory and Computation*, **2015**, 11, 2421-8	6.4	27
53	Estimating diffusivity along a reaction coordinate in the high friction limit: Insights on pulse times in laser-induced nucleation. *Journal of Chemical Physics*, **2009**, 131, 224112	3.9	26
52	Biasing a transition state search to locate multiple reaction pathways. *Journal of Chemical Physics*, **2003**, 118, 9533-9541	3.9	26
51	Transition-State Theory, Dynamics, and Narrow Time Scale Separation in the Rate-Promoting Vibrations Model of Enzyme Catalysis. *Journal of Chemical Theory and Computation*, **2010**, 6, 1447-54	6.4	25
50	p(TP|q) peak maximization: Necessary but not sufficient for reaction coordinate accuracy. *Chemical Physics Letters*, **2010**, 494, 100-103	2.5	24

49	Reexamining the evidence for proton transfers in ethylene polymerization. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, E4160-1	11.5	23
48	Rate constants from the reaction path Hamiltonian. I. Reactive flux simulations for dynamically correct rates. *Journal of Chemical Physics*, **2004**, 121, 4453-60	3.9	23
47	On the coupling between slow diffusion transport and barrier crossing in nucleation. *Journal of Chemical Physics*, **2011**, 135, 044107	3.9	22
46	Mechanisms and Nucleation Rate of Methane Hydrate by Dynamical Nonequilibrium Molecular Dynamics. *Journal of Physical Chemistry C*, **2017**, 121, 24223-24234	3.8	21
45	Salting out the polar polymorph: analysis by alchemical solvent transformation. *Journal of Chemical Physics*, **2014**, 140, 014501	3.9	20
44	Energetic and entropic components of the Tolman length for mW and TIP4P/2005 water nanodroplets. *Journal of Chemical Physics*, **2016**, 145, 204703	3.9	20
43	Computational Support for Phillips Catalyst Initiation via Cr□ Bond Homolysis in a Chromacyclopentane Site. *ACS Catalysis*, **2018**, 8, 1728-1733	13.1	18
42	Water-catalyzed activation of H2O2 by methyltrioxorhenium: a combined computational-experimental study. *Inorganic Chemistry*, **2013**, 52, 13904-17	5.1	17
41	Polymorph specific RMSD local order parameters for molecular crystals and nuclei: □ □ and □glycine. *Journal of Chemical Physics*, **2011**, 135, 134101	3.9	17
40	Rate constants from the reaction path Hamiltonian. II. Nonseparable semiclassical transition state theory. *Journal of Chemical Physics*, **2004**, 121, 4461-6	3.9	17
39	Accelerated Nucleation Due to Trace Additives: A Fluctuating Coverage Model. *Journal of Physical Chemistry B*, **2016**, 120, 1679-84	3.4	16
38	Solvent and additive interactions as determinants in the nucleation pathway: general discussion. *Faraday Discussions*, **2015**, 179, 383-420	3.6	15
37	Nucleation near the eutectic point in a Potts-lattice gas model. *Journal of Chemical Physics*, **2014**, 140, 084111	3.9	15
36	Transition path sampling for discrete master equations with absorbing states. *Journal of Chemical Physics*, **2012**, 137, 094106	3.9	15
35	A design equation for low dosage additives that accelerate nucleation. *Faraday Discussions*, **2015**, 179, 329-41	3.6	14
34	Site-averaged kinetics for catalysts on amorphous supports: an importance learning algorithm. *Reaction Chemistry and Engineering*, **2020**, 5, 77-86	4.9	14
33	In Silico Crystal Growth Rate Prediction for NaCl from Aqueous Solution. *Crystal Growth and Design*, **2018**, 18, 6302-6306	3.5	12
32	Modeling Step Velocities and Edge Surface Structures during Growth of Non-Centrosymmetric Crystals. *Crystal Growth and Design*, **2017**, 17, 2066-2080	3.5	11

31	Grafting metal complexes onto amorphous supports: from elementary steps to catalyst site populations via kernel regression. *Reaction Chemistry and Engineering*, **2020**, 5, 66-76	4.9	11
30	Mitosis method for directly calculating the interfacial free energy of nuclei. *Molecular Simulation*, **2010**, 36, 498-504	2	8
29	Soluble Oligomeric Nucleants: Simulations of Chain Length, Binding Strength, and Volume Fraction Effects. *Journal of Physical Chemistry Letters*, **2017**, 8, 5815-5820	6.4	7
28	Comment on "Toward identification of the reaction coordinate directly from the transition state ensemble using the kernel PCA method". *Journal of Physical Chemistry B*, **2011**, 115, 12671-3; discussion 12674-5	3.4	7
27	Tandem Catalysts for Polyethylene Upcycling: A Simple Kinetic Model. *Journal of Physical Chemistry A*, **2020**, 124, 3935-3942	2.8	6
26	Diabat Interpolation for Polymorph Free-Energy Differences. *Journal of Physical Chemistry Letters*, **2017**, 8, 655-660	6.4	5
25	Performing solvation free energy calculations in LAMMPS using the decoupling approach. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 641-646	4.2	5
24	A Career in Catalysis: Alexis T. Bell. *ACS Catalysis*, **2017**, 7, 8628-8640	13.1	4
23	Solvent reaction coordinate for an S2 reaction. *Journal of Chemical Physics*, **2020**, 153, 024103	3.9	4
22	Critical length of a one-dimensional nucleus. *Journal of Chemical Physics*, **2016**, 145, 211916	3.9	4
21	Size-Controlled Nanoparticles Embedded in a Mesoporous Architecture Leading to Efficient and Selective Hydrogenolysis of Polyolefins.. *Journal of the American Chemical Society*, **2022**,	16.4	4
20	Secondary effectiveness factors for catalytic reactions in series: extension to slab, cylindrical, and spherical geometries. *Reaction Chemistry and Engineering*, **2020**, 5, 2003-2008	4.9	3
19	Secondary Effectiveness Factors and Solubility Effects for Catalytic Reactions in Series. *ACS Catalysis*, **2020**, 10, 4319-4325	13.1	3
18	Nonequilibrium Kink Density from One-Dimensional Nucleation for Step Velocity Predictions. *Crystal Growth and Design*, **2018**, 18, 723-727	3.5	3
17	How fluxional reactants limit the accuracy/efficiency of infrequent metadynamics. *Journal of Chemical Physics*, **2020**, 153, 054125	3.9	3
16	Headspace diffusion limitations on heterogeneous catalysis in unstirred batch reactors. *Chemical Engineering Science*, **2012**, 71, 367-374	4.4	2
15	Importance learning estimator for the site-averaged turnover frequency of a disordered solid catalyst. *Journal of Chemical Physics*, **2020**, 153, 244120	3.9	2
14	Free energies of crystals computed using Einstein crystal with fixed center of mass and differing spring constants. *Journal of Chemical Physics*, **2021**, 154, 164509	3.9	2

13	Coupled Population Balance and Species Balance Models of Crystallization: Analytic Solutions and Data Fits. *Crystal Growth and Design*, **2021**, 21, 227-234	3.5	2
12	Predicted Properties of Active Catalyst Sites on Amorphous Silica: Impact of Silica Preoptimization Protocol. *Industrial & Engineering Chemistry Research*, **2021**, 60, 12834-12846	3.9	2
11	Nucleation in complex multi-component and multi-phase systems: general discussion. *Faraday Discussions*, **2015**, 179, 503-42	3.6	1
10	Reactive flux **2017**, 335-362		1
9	Diabat method for polymorph free energies: Extension to molecular crystals. *Journal of Chemical Physics*, **2020**, 153, 244105	3.9	1
8	Multiscale Models for Fibril Formation: Rare Events Methods, Microkinetic Models, and Population Balances. *Life*, **2021**, 11,	3	1
7	The overdamped transmission coefficient: Recovering the true mean first passage time from an inaccurate reaction coordinate. *Journal of Chemical Physics*, **2019**, 151, 184108	3.9	1
6	Solid-solid phase equilibria in the NaCl-KCl system. *Journal of Chemical Physics*, **2020**, 152, 144109	3.9	1
5	Crystallization with Sinusoidal Modulation of Stirrer Speed: Frequency Response Analysis and Secondary Nucleation Kinetics. *Crystal Growth and Design*, **2021**, 21, 235-242	3.5	1
4	Gibbs free-energy differences between polymorphs via a diabat approach. *Journal of Chemical Physics*, **2018**, 149, 214106	3.9	1
3	Modeling the Structural Heterogeneity of Vicinal Silanols and Its Effects on TiCl4 Grafting onto Amorphous Silica. *Chemistry of Materials*, **2022**, 34, 3920-3930	9.6	1
2	Absolute chemical potentials for complex molecules in fluid phases: A centroid reference for predicting phase equilibria. *Journal of Chemical Physics*, **2020**, 153, 214504	3.9	0
1	Crystal nucleation: Rare made common and captured by Raman.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119, e2204971119	11.5	0