Titus S Van Erp

List of Publications by Year
in descending order

63 papers	2,443 citations	201385 27 h-index	205818 48 g-index
65 all docs	65 docs citations	65 times ranked	2214 citing authors

#	Article	IF	Citations
1	A novel path sampling method for the calculation of rate constants. Journal of Chemical Physics, 2003, 118, 7762-7774.	1.2	434
2	Elaborating transition interface sampling methods. Journal of Computational Physics, 2005, 205, 157-181.	1.9	229
3	Rate constants for diffusive processes by partial path sampling. Journal of Chemical Physics, 2004, 120, 4055-4065.	1.2	155
4	Reaction Rate Calculation by Parallel Path Swapping. Physical Review Letters, 2007, 98, 268301.	2.9	91
5	Ab initio molecular dynamics study of liquid methanol. Chemical Physics Letters, 2003, 367, 617-624.	1.2	79
6	²⁹Si NMR and UVâ^'Raman Investigation of Initial Oligomerization Reaction Pathways in Acid-Catalyzed Silica Solâ^'Gel Chemistry. Journal of Physical Chemistry C, 2011, 115, 3562-3571.	1.5	72
7	Hydration of methanol in water. A DFT-based molecular dynamics study. Chemical Physics Letters, 2001, 333, 290-296.	1.2	68
8	Investigating rare events by transition interface sampling. Physica A: Statistical Mechanics and Its Applications, 2004, 340, 395-401.	1.2	68
9	Bubbles and denaturation in DNA. European Physical Journal E, 2006, 20, 421-434.	0.7	64
10	Can One Predict DNA Transcription Start Sites by Studying Bubbles?. Physical Review Letters, 2005, 95, 218104.	2.9	62
11	Investigation of the Mechanism of Colloidal Silicaliteâ€1 Crystallization by Using DLS, SAXS, and ²⁹Si NMR Spectroscopy. Chemistry - A European Journal, 2010, 16, 2764-2774.	1.7	60
12	Ab initiomolecular dynamics study of aqueous solvation of ethanol and ethylene. Journal of Chemical Physics, 2003, 118, 8831-8840.	1.2	59
13	Continuous Synthesis Process of Hexagonal Nanoplates of P6m Ordered Mesoporous Silica. Journal of the American Chemical Society, 2011, 133, 13737-13745.	6.6	54
14	Enantioselective adsorption of ibuprofen and lysine in metalâ€“organic frameworks. Chemical Communications, 2014, 50, 10849.	2.2	52
15	Local initiation conditions for water autoionization. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E4569-E4576.	3.3	52
16	Foundations and latest advances in replica exchange transition interface sampling. Journal of Chemical Physics, 2017, 147, 152722.	1.2	43
17	Efficient Numerical Reconstruction of Protein Folding Kinetics with Partial Path Sampling and Pathlike Variables. Physical Review Letters, 2013, 110, 108106.	2.9	41
18	Efficiency analysis of reaction rate calculation methods using analytical models I: The two-dimensional sharp barrier. Journal of Chemical Physics, 2006, 125, 174106.	1.2	39

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19	Simultaneous computation of free energies and kinetics of rare events. Physical Review E, 2005, 71, 056709.	0.8	38
20	Pinning and phonon localization in Frenkel-Kontorova models on quasiperiodic substrates. Physical Review B, 1999, 60, 6522-6528.	1.1	36
21	Enantioselective Adsorption in Achiral Zeolites. Angewandte Chemie - International Edition, 2010, 49, 3010-3013.	7.2	36
22	A standardization for BET fitting of adsorption isotherms. Microporous and Mesoporous Materials, 2011, 145, 188-193.	2.2	35
23	Low barriers for hydrogen diffusion in sII clathrate. Physical Chemistry Chemical Physics, 2015, 17, 13808-13812.	1.3	34
24	Density Functional Theory Study on the Interactions of Metal Ions with Long Chain Deprotonated Carboxylic Acids. Journal of Physical Chemistry A, 2015, 119, 10195-10203.	1.1	33
25	PyRETIS: A wellâ€done, mediumâ€sized python library for rare events. Journal of Computational Chemistry, 2017, 38, 2439-2451.	1.5	30
26	Ab Initio Molecular Dynamics Study on the Interactions between Carboxylate Ions and Metal Ions in Water. Journal of Physical Chemistry B, 2015, 119, 10710-10719.	1.2	28
27	Proton-Assisted Ethylene Hydration in Aqueous Solution. Angewandte Chemie - International Edition, 2004, 43, 1660-1662.	7.2	27
28	Rare event simulations reveal subtle key steps in aqueous silicate condensation. Physical Chemistry Chemical Physics, 2017, 19, 13361-13371.	1.3	27
29	Analyzing Complex Reaction Mechanisms Using Path Sampling. Journal of Chemical Theory and Computation, 2016, 12, 5398-5410.	2.3	25
30	Molecular Structure and Solubility Determination of Asphaltenes. Energy & Fuels, 2019, 33, 8259-8270.	2.5	22
31	Investigation of Nanoparticles Occurring in the Colloidal Silicalite-1 Zeolite Crystallization Process Using Dissolution Experiments. Chemistry of Materials, 2010, 22, 3619-3629.	3.2	21
32	Molecular Dynamics in Principal Component Space. Journal of Physical Chemistry B, 2012, 116, 8350-8354.	1.2	21
33	Fast Decorrelating Monte Carlo Moves for Efficient Path Sampling. Journal of Physical Chemistry Letters, 2017, 8, 4456-4460.	2.1	21
34	PyRETIS 2: An improbability drive for rare events. Journal of Computational Chemistry, 2020, 41, 370-377.	1.5	20
35	A test on reactive force fields for the study of silica dimerization reactions. Journal of Chemical Physics, 2015, 143, 184113.	1.2	19
36	Heat and Mass Transfer across Interfaces in Complex Nanogeometries. Physical Review Letters, 2015, 114, 065901.	2.9	19

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37	Diffusion of gas mixtures in the sI hydrate structure. Journal of Chemical Physics, 2018, 148, 214701.	1.2	17
38	Enantioselective Adsorption Characteristics of Aluminum-Substituted MFI Zeolites. Chemistry of Materials, 2010, 22, 4591-4601.	3.2	15
39	Effective Monte Carlo Scheme for Multicomponent Gas Adsorption and Enantioselectivity in Nanoporous Materials. Journal of Physical Chemistry Letters, 2010, 1, 2154-2158.	2.1	14
40	The dynamics of the DNA denaturation transition. Europhysics Letters, 2012, 98, 48004.	0.7	12
41	Adsorption of Polar Enantiomers in Achiral Zeolites. Journal of Physical Chemistry C, 2013, 117, 1524-1530.	1.5	12
42	Exact non-Markovian permeability from rare event simulations. Physical Review Research, 2021, 3, .	1.3	12
43	Prospects of transition interface sampling simulations for the theoretical study of zeolite synthesis. Physical Chemistry Chemical Physics, 2007, 9, 1044.	1.3	11
44	Kinetics of intermediate-mediated self-assembly in nanosized materials: A generic model. Journal of Chemical Physics, 2010, 132, 164701.	1.2	11
45	Efficient path sampling on multiple reaction channels. Computer Physics Communications, 2008, 179, 34-40.	3.0	10
46	van ErpetÂal.Reply:. Physical Review Letters, 2006, 96, .	2.9	9
47	Permeation Rates of Oxygen through a Lipid Bilayer Using Replica Exchange Transition Interface Sampling. Journal of Physical Chemistry B, 2021, 125, 193-201.	1.2	9
48	van ErpetÂal.Reply:. Physical Review Letters, 2006, 97, .	2.9	8
49	On the relation between the Langmuir and thermodynamic flux equations. Frontiers in Physics, 2014, 1, .	1.0	7
50	Aubry transition studied by direct evaluation of the modulation functions of infinite incommensurate systems. Europhysics Letters, 2002, 59, 330-336.	0.7	6
51	On the application of chiral amplification via adsorption. Chemical Engineering Science, 2010, 65, 6478-6485.	1.9	6
52	A procedure to find thermodynamic equilibrium constants for CO₂ and CH₄ adsorption on activated carbon. Physical Chemistry Chemical Physics, 2015, 17, 8223-8230.	1.3	6
53	Breakdown of Lindstedt expansion for chaotic maps. Journal of Mathematical Physics, 2005, 46, 102702.	0.5	5
54	Comment on â€œA generalized Langevin formalism of complete DNA melting transition" by Das T. and Chakraborty S.. Europhysics Letters, 2009, 85, 68003.	0.7	5

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55	Gluing Potential Energy Surfaces with Rare Event Simulations. Journal of Chemical Theory and Computation, 2015, 11, 2440-2450.	2.3	5
56	Mesoscopic modeling of DNA denaturation rates: Sequence dependence and experimental comparison. Journal of Chemical Physics, 2015, 142, 235101.	1.2	5
57	Structural transitions and phonon localization in frenkel kontorova models with quasi-periodic potentials. Ferroelectrics, 2001, 250, 421-424.	0.3	3
58	Enantiomeric Adsorption of Lactic Acid Mixtures in Achiral Zeolites. Journal of Physical Chemistry C, 2014, 118, 14991-14997.	1.5	3
59	Thin film breakage in oilâ€“inâ€“water emulsions, a multidisciplinary study. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 632, 127808.	2.3	3
60	Multiscale partial charge estimation on graphene for neutral, doped and charged flakes. Physical Chemistry Chemical Physics, 2018, 20, 20678-20687.	1.3	2
61	Teaching complex molecular simulation algorithms: Using selfâ€evaluation to tailor webâ€based exercises at an individual level. Computer Applications in Engineering Education, 2020, 28, 779-791.	2.2	2
62	Improving the mesoscopic modeling of DNA denaturation dynamics. Physical Biology, 2018, 15, 066001.	0.8	1
63	The role of pressure and defects in the wurtzite to rock salt transition in cadmium selenide. Physical Chemistry Chemical Physics, 2022, 24, 8378-8386.	1.3	1