

Upakarasamy Lourderaj

List of Publications by Year in descending order

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41
papers

1,384
citations

516215

16
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329751

37
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44
all docs

44
docs citations

44
times ranked

1340
citing authors

#	ARTICLE	IF	CITATIONS
1	Imaging Nucleophilic Substitution Dynamics. <i>Science</i> , 2008, 319, 183-186.	6.0	307
2	Classical trajectory simulations of post-transition state dynamics. <i>International Reviews in Physical Chemistry</i> , 2008, 27, 361-403.	0.9	147
3	Theoretical and Computational Studies of Non-RRKM Unimolecular Dynamics. <i>Journal of Physical Chemistry A</i> , 2009, 113, 2236-2253.	1.1	146
4	A Direct Dynamics Trajectory Study of $F + CH_3OOH$ Reactive Collisions Reveals a Major Non-IRC Reaction Path. <i>Journal of the American Chemical Society</i> , 2007, 129, 9976-9985.	6.6	139
5	The VENUS/NWChem software package. Tight coupling between chemical dynamics simulations and electronic structure theory. <i>Computer Physics Communications</i> , 2014, 185, 1074-1080.	3.0	93
6	Simulation studies of the $Cl^- + CH_3I$ SN2 nucleophilic substitution reaction: Comparison with ion imaging experiments. <i>Journal of Chemical Physics</i> , 2013, 138, 114309.	1.2	55
7	Isolation and Characterization of Regioisomers of Pyrazole-Based Palladacycles and Their Use in α -Alkylation of Ketones Using Alcohols. <i>Organometallics</i> , 2017, 36, 3343-3351.	1.1	49
8	Direct dynamics simulations using Hessian-based predictor-corrector integration algorithms. <i>Journal of Chemical Physics</i> , 2007, 126, 044105.	1.2	45
9	Chemical Dynamics Simulations of Energy Transfer in Collisions of Protonated Peptide Ions with a Perfluorinated Alkylthiol Self-Assembled Monolayer Surface. <i>Journal of Physical Chemistry C</i> , 2008, 112, 9377-9386.	1.5	35
10	Cyclohexane Isomerization. Unimolecular Dynamics of the Twist-Boat Intermediate. <i>Journal of Physical Chemistry A</i> , 2009, 113, 4570-4580.	1.1	35
11	Potential energy surface and unimolecular dynamics of stretched n-butane. <i>Journal of Chemical Physics</i> , 2008, 129, 094701.	1.2	34
12	Theoretical Investigation of Mechanisms for the Gas-Phase Unimolecular Decomposition of DMMP. <i>Journal of Physical Chemistry A</i> , 2009, 113, 13762-13771.	1.1	33
13	Quantum Chemical Calculations of the $Cl + CH_3I \rightarrow CH_3Cl + I$ Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1976-1984.	1.1	29
14	Conformational Control and Photoenolization of Pyridine-3-carboxaldehydes in the Solid State: π -Stabilization of Photoenols via Hydrogen Bonding and Electronic Control. <i>Journal of Organic Chemistry</i> , 2003, 68, 3446-3453.	1.7	25
15	Ground and Excited States of the Monomer and Dimer of Certain Carboxylic Acids. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2709-2717.	1.1	25
16	Mechanisms and dynamics of protonation and lithiation of ferrocene. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 22204-22209.	1.3	18
17	Palladium-catalyzed selective C-C bond cleavage and stereoselective alkenylation between cyclopropanol and 1,3-diyne: one-step synthesis of diverse conjugated enynes. <i>Chemical Science</i> , 2022, 13, 2692-2700.	3.7	17
18	Can reactions follow non-traditional second-order saddle pathways avoiding transition states?. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 12837-12842.	1.3	16

#	ARTICLE	IF	CITATIONS
19	Determination of Stability and Degradation in Polysilanes by an Electronic Mechanism. Journal of Physical Chemistry B, 2005, 109, 15860-15867.	1.2	13
20	Ab Initio Quantum Chemical Investigation of the Ground and Excited States of Salicylic Acid Dimer. Journal of Physical Chemistry A, 2006, 110, 12662-12669.	1.1	13
21	Chemical Dynamics Simulations of CO ₂ in the Ground and First Excited Bend States Colliding with a Perfluorinated Self-Assembled Monolayer. Journal of Physical Chemistry C, 2010, 114, 18455-18464.	1.5	12
22	Time-dependent density functional theoretical study of low lying excited states of F2. Chemical Physics Letters, 2002, 366, 88-94.	1.2	11
23	Transition between [<i>R</i>]- and [<i>S</i>]-stereoisomers without bond breaking. Physical Chemistry Chemical Physics, 2020, 22, 14983-14991.	1.3	11
24	HeH ⁺ Collisions with H ₂ : Rotationally Inelastic Cross Sections and Rate Coefficients from Quantum Dynamics at Interstellar Temperatures. Journal of Physical Chemistry A, 2022, 126, 2244-2261.	1.1	11
25	Time-Dependent Density Functional Theoretical Investigation of Photoinduced Excited-State Intramolecular Dual Proton Transfer in Diformyl Dipyrrromethanes. Journal of Physical Chemistry A, 2016, 120, 9894-9906.	1.1	10
26	Quantum chemical investigation of the thermal denitrogenation of 1-pyrazoline. Physical Chemistry Chemical Physics, 2017, 19, 27468-27477.	1.3	8
27	Theoretical investigation of the isomerization pathways of diazenes: torsion vs. inversion. Physical Chemistry Chemical Physics, 2019, 21, 15678-15685.	1.3	8
28	Modeling the formaldehyde-graphene interaction using a formaldehyde-pyrene system. Physical Chemistry Chemical Physics, 2013, 15, 17479.	1.3	6
29	Dynamics of a gas-phase SNAr reaction: non-concerted mechanism despite the Meisenheimer complex being a transition state. Physical Chemistry Chemical Physics, 2020, 22, 26562-26567.	1.3	6
30	Machine Learning in Chemical Dynamics. Resonance, 2020, 25, 59-75.	0.2	5
31	Second-order Saddle Dynamics in Isomerization Reaction. Regular and Chaotic Dynamics, 2021, 26, 119-130.	0.3	5
32	Ab initio potential energy surface for HeF2 in its ground electronic state. Chemical Physics, 2005, 308, 277-284.	0.9	3
33	Representing and Selecting Vibrational Angular Momentum States for Quasiclassical Trajectory Chemical Dynamics Simulations. Journal of Physical Chemistry A, 2007, 111, 10292-10301.	1.1	3
34	Stereomutation in Tetracoordinate Centers via Stabilization of Planar Tetracoordinated Systems. Atoms, 2021, 9, 79.	0.7	3
35	Stability in polysilanes for light emitting diodes. Computational Materials Science, 2005, 33, 206-211.	1.4	2
36	Synthesis and computational aspects of Al(II) and Ga(II) dihalides based on an amidinate scaffold. Dalton Transactions, 2022, 51, 4898-4902.	1.6	2

