Upakarasamy Lourderaj

List of Publications by Year
in descending order

41 papers	1,384 citations	516215 16 h-index	329751 37 g-index
44 all docs	44 docs citations	44 times ranked	1340 citing authors

#	Article	IF	Citations
1	Palladium-catalyzed selective Câ€“C bond cleavage and stereoselective alkenylation between cyclopropanol and 1,3-diyne: one-step synthesis of diverse conjugated enynes. Chemical Science, 2022, 13, 2692-2700.	3.7	17
2	Synthesis and computational aspects of Al(<scp>ii</scp>)â€“Al(<scp>ii</scp>) and Ga(<scp>ii</scp>)â€“Ga(<scp>ii</scp>) dihalides based on an amidinate scaffold. Dalton Transactions, 2022, 51, 4898-4902.	1.6	2
3	HeH⁺ Collisions with H₂: 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
4	Mechanism and dynamics of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:msub><mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:mi mathvariant="normal">H</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub><mml:msubsup><mm mathvariant="normal">N</mml:mi><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow><mml:mrow><mml:mo>â^'</mml:m CCl4 halophilic reaction. International Journal of Mass Spectrometry, 2021, 459, 116470.	0.7	0
5	Second-order Saddle Dynamics in Isomerization Reaction. Regular and Chaotic Dynamics, 2021, 26, 119-130.	0.3	5
6	Stereomutation in Tetracoordinate Centers via Stabilization of Planar Tetracoordinated Systems. Atoms, 2021, 9, 79.	0.7	3
7	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
8	Transition between [R]- and [S]-stereoisomers without bond breaking. Physical Chemistry Chemical Physics, 2020, 22, 14983-14991.	1.3	11
9	Machine Learning in Chemical Dynamics. Resonance, 2020, 25, 59-75.	0.2	5
10	Can reactions follow non-traditional second-order saddle pathways avoiding transition states?. Physical Chemistry Chemical Physics, 2019, 21, 12837-12842.	1.3	16
11	Theoretical investigation of the isomerization pathways of diazenes: torsion vs. inversion. Physical Chemistry Chemical Physics, 2019, 21, 15678-15685.	1.3	8
12	Computational Studies on the Excited-State Intramolecular Proton Transfer in Five-Membered-Ring Hydrogen-Bonded Systems. , 2019, , 155-178.		1
13	Classical Dynamics Simulations of Dissociation of Protonated Tryptophan in the Gas Phase. Journal of Physical Chemistry A, 2017, 121, 4389-4396.	1.1	1
14	Quantum chemical investigation of the thermal denitrogenation of 1-pyrazoline. Physical Chemistry Chemical Physics, 2017, 19, 27468-27477.	1.3	8
15	Isolation and Characterization of Regioisomers of Pyrazole-Based Palladacycles and Their Use in Î±-Alkylation of Ketones Using Alcohols. Organometallics, 2017, 36, 3343-3351.	1.1	49
16	Time-Dependent Density Functional Theoretical Investigation of Photoinduced Excited-State Intramolecular Dual Proton Transfer in Diformyl Dipyrromethanes. Journal of Physical Chemistry A, 2016, 120, 9894-9906.	1.1	10
17	Mechanisms and dynamics of protonation and lithiation of ferrocene. Physical Chemistry Chemical Physics, 2015, 17, 22204-22209.	1.3	18
18	The VENUS/NWChem software package. Tight coupling between chemical dynamics simulations and electronic structure theory. Computer Physics Communications, 2014, 185, 1074-1080.	3.0	93

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19	Modeling the formaldehydeâ€“graphene interaction using a formaldehydeâ€“pyrene system. Physical Chemistry Chemical Physics, 2013, 15, 17479.	1.3	6
20	A Load-Balancing Force Decomposition Scheme for Parallel Simulation of Chemical Dynamics with Multiple Inter-atomic Force Models. , 2013, , .		0
21	Simulation studies of the Clâ^' + CH3I SN2 nucleophilic substitution reaction: Comparison with ion imaging experiments. Journal of Chemical Physics, 2013, 138, 114309.	1.2	55
22	Chemical Dynamics Simulations of CO₂in 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
23	Theoretical and Computational Studies of Non-RRKM Unimolecular Dynamics. Journal of Physical Chemistry A, 2009, 113, 2236-2253.	1.1	146
24	Quantum Chemical Calculations of the Cl^{â^'} + CH₃I â†' CH₃Cl + I^{â^'} Potential Energy Surface. Journal of Physical Chemistry A, 2009, 113, 1976-1984.	1.1	29
25	Theoretical Investigation of Mechanisms for the Gas-Phase Unimolecular Decomposition of DMMP. Journal of Physical Chemistry A, 2009, 113, 13762-13771.	1.1	33
26	Cyclohexane Isomerization. Unimolecular Dynamics of the Twist-Boat Intermediate. Journal of Physical Chemistry A, 2009, 113, 4570-4580.	1.1	35
27	Classical trajectory simulations of post-transition state dynamics. International Reviews in Physical Chemistry, 2008, 27, 361-403.	0.9	147
28	Imaging Nucleophilic Substitution Dynamics. Science, 2008, 319, 183-186.	6.0	307
29	Potential energy surface and unimolecular dynamics of stretched n-butane. Journal of Chemical Physics, 2008, 129, 094701.	1.2	34
30	Chemical Dynamics Simulations of Energy Transfer in Collisions of Protonated Peptideâ^'Ions with a Perfluorinated Alkylthiol Self-Assembled Monolayer Surface. Journal of Physical Chemistry C, 2008, 112, 9377-9386.	1.5	35
31	Direct dynamics simulations using Hessian-based predictor-corrector integration algorithms. Journal of Chemical Physics, 2007, 126, 044105.	1.2	45
32	A Direct Dynamics Trajectory Study of F⁻+ CH₃OOH Reactive Collisions Reveals a Major Non-IRC Reaction Path. Journal of the American Chemical Society, 2007, 129, 9976-9985.	6.6	139
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	Ground and Excited States of the Monomer and Dimer of Certain Carboxylic Acids. Journal of Physical Chemistry A, 2006, 110, 2709-2717.	1.1	25
35	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
36	Ab initio potential energy surface for HeF2 in its ground electronic state. Chemical Physics, 2005, 308, 277-284.	0.9	3

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37	Determination of Stability and Degradation in Polysilanes by an Electronic Mechanism. Journal of Physical Chemistry B, 2005, 109, 15860-15867.	1.2	13
38	Stability in polysilanes for light emitting diodes. Computational Materials Science, 2005, 33, 206-211.	1.4	2
39	Conformational Control and Photoenolization of Pyridine-3-carboxaldehydes in the Solid State:Â Stabilization of Photoenols via Hydrogen Bonding and Electronic Control. Journal of Organic Chemistry, 2003, 68, 3446-3453.	1.7	25
40	Time-dependent density functional theoretical study of low lying excited states of F2. Chemical Physics Letters, 2002, 366, 88-94.	1.2	11
41	Influence of second-order saddles on reaction mechanisms. Faraday Discussions, 0, , .	1.6	2