Noelia Faginas Lago

List of Publications by Year
in descending order

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149 papers	3,660 citations	116194 36 h-index	198040 52 g-index
152 all docs	152 docs citations	152 times ranked	2242 citing authors

#	Article	IF	Citations
1	Quantum Mechanical Simulations of the Radicalâ€“Radical Chemistry on Icy Surfaces. Astrophysical Journal, Supplement Series, 2022, 259, 39.	3.0	24
2	Semiempirical Potential in Kinetics Calculations on the HC3N + CN Reaction. Molecules, 2022, 27, 2297.	1.7	3
3	Unsaturated Dinitriles Formation Routes in Extraterrestrial Environments: A Combined Experimental and Theoretical Investigation of the Reaction between Cyano Radicals and Cyanoethene (C₂H₃CN). Journal of Physical Chemistry A, 2022, 126, 3569-3582.	1.1	13
4	A Computational Study on the Attack of Nitrogen and Oxygen Atoms to Toluene. Lecture Notes in Computer Science, 2021, , 620-631.	1.0	6
5	Intermolecular Forces for the Interaction of H$$_{2}$$Oâ€“Graphtriyne Membrane: Contribution of Induction Effects. Lecture Notes in Computer Science, 2021, , 426-438.	1.0	0
6	A Minimal Model of Potential Energy Surface for the CO2 â€“ CO System. Lecture Notes in Computer Science, 2021, , 351-362.	1.0	1
7	Classification of Biomolecules byÂInvariant Shape Coordinates andÂDeformation Indexes. Lecture Notes in Computer Science, 2021, , 363-374.	1.0	0
8	A New Method for Binary Classification of Proteins with Machine Learning. Lecture Notes in Computer Science, 2021, , 388-397.	1.0	7
9	FAUST. II. Discovery of a Secondary Outflow in IRAS 15398â˜3359: Variability in Outflow Direction during the Earliest Stage of Star Formation?. Astrophysical Journal, 2021, 910, 11.	1.6	19
10	Interaction of HCO+ Cations With Interstellar Negative Grains. Quantum Chemical Investigation and Astrophysical Implications. Frontiers in Astronomy and Space Sciences, 2021, 8, .	1.1	5
11	Confinement of $$hbox {CO}_{2}$$ inside carbon nanotubes. European Physical Journal D, 2021, 75, 1.	0.6	5
12	Deactivation dynamics of carbon dioxide in gas phase at thermal and moderately high temperature regimes. Chemical Physics Letters, 2021, 779, 138850.	1.2	0
13	Structures and Properties of Known and Postulated Interstellar Cations. Astrophysical Journal, Supplement Series, 2021, 256, 35.	3.0	4
14	Grand Canonical Monte Carlo Simulations to Determine the Optimal Interlayer Distance of a Graphene Slit-Shaped Pore for Adsorption of Methane, Hydrogen and their Equimolar Mixture. Nanomaterials, 2021, 11, 2534.	1.9	5
15	Long-Range Complex in the HC$$_{3}$$N + CN Potential Energy Surface: Ab Initio Calculations and Intermolecular Potential. Lecture Notes in Computer Science, 2021, , 413-425.	1.0	2
16	The Reaction N(²D) + CH₃CCH (Methylacetylene): A Combined Crossed Molecular Beams and Theoretical Investigation and Implications for the Atmosphere of Titan. Journal of Physical Chemistry A, 2021, 125, 8846-8859.	1.1	12
17	Toward a Generalized HÃ¼ckel Rule: The Electronic Structure of Carbon Nanocones. Journal of Physical Chemistry A, 2021, 125, 9819-9825.	1.1	8
18	Distributed Gaussian orbitals for molecular calculations: application to simple systems. Molecular Physics, 2020, 118, 1615646.	0.8	2

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19	A novel intermolecular potential to describe the interaction between the azide anion and carbon nanotubes. Diamond and Related Materials, 2020, 101, 107533.	1.8	6
20	Gas-phase formation of acetaldehyde: review and new theoretical computations. Monthly Notices of the Royal Astronomical Society, 2020, 499, 5547-5561.	1.6	30
21	Two-dimensional diamine-linked covalent organic frameworks for CO₂/N₂ capture and separation: theoretical modeling and simulations. Physical Chemistry Chemical Physics, 2020, 22, 25918-25929.	1.3	16
22	A Computational Study of the Reaction Cyanoacetylene and Cyano Radical Leading to 2-Butynedinitrile and Hydrogen Radical. Lecture Notes in Computer Science, 2020, , 707-716.	1.0	3
23	A Computational Study on the Insertion of N(2D) into a Câ€”H or Câ€”C Bond: The Reactions of N(2D) with Benzene and Toluene and Their Implications on the Chemistry of Titan. Lecture Notes in Computer Science, 2020, , 744-755.	1.0	7
24	Carbon Capture and Separation from CO2/N2/H2O Gaseous Mixtures in Bilayer Graphtriyne: A Molecular Dynamics Study. Lecture Notes in Computer Science, 2020, , 489-501.	1.0	4
25	Gas Adsorption on Graphtriyne Membrane: Impact of the Induction Interaction Term on the Computational Cost. Lecture Notes in Computer Science, 2020, , 513-525.	1.0	1
26	Binary Classification of Proteins by a Machine Learning Approach. Lecture Notes in Computer Science, 2020, , 549-558.	1.0	13
27	The quest for a detailed comprehension of elementary reactions in combustion: A crossed molecular beam study of the O(3P) reactions with unsaturated C4 hydrocarbons. AIP Conference Proceedings, 2020, , .	0.3	0
28	Classification of Shapes and Deformations of Large Systems by Invariant Coordinates. Lecture Notes in Computer Science, 2020, , 538-548.	1.0	0
29	The Fragmentation Dynamics of Simple Organic Molecules of Astrochemical Interest Interacting with VUV Photons. ACS Earth and Space Chemistry, 2019, 3, 1862-1872.	1.2	3
30	Molecular Simulations of CO$$_{2}$$/N$$_{2}$$/H$$_{2}$$O Gaseous Mixture Separation in Graphtriyne Membrane. Lecture Notes in Computer Science, 2019, , 374-387.	1.0	5
31	A Computational Study of the Reaction N(2D)Â+ÂC6H6 Leading to Pyridine and Phenylnitrene. Lecture Notes in Computer Science, 2019, , 316-324.	1.0	10
32	Electronic Structure and Kinetics Calculations for the Si+SH Reaction, a Possible Route of SiS Formation in Star-Forming Regions. Lecture Notes in Computer Science, 2019, , 306-315.	1.0	4
33	The Invariance Approach to Structure and Dynamics: Classical Hyperspherical Coordinates. Lecture Notes in Computer Science, 2019, , 428-438.	1.0	5
34	Flexibility in the Graphene Sheet: The Influence on Gas Adsorption from Molecular Dynamics Studies. Journal of Physical Chemistry C, 2019, 123, 28035-28047.	1.5	14
35	Angular Distribution of Ion Products in the Double Photoionization of Propylene Oxide. Frontiers in Chemistry, 2019, 7, 621.	1.8	6
36	Interstellar Formamide (NH₂CHO), a Key Prebiotic Precursor. ACS Earth and Space Chemistry, 2019, 3, 2122-2137.	1.2	57

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37	Reactivity of HCO with CH₃ and NH₂ on Water Ice Surfaces. A Comprehensive Accurate Quantum Chemistry Study. ACS Earth and Space Chemistry, 2019, 3, 2158-2170.	1.2	55
38	The HH 212 Interstellar Laboratory: Astrochemistry as a Tool To Reveal Protostellar Disks on Solar System Scales around a Rising Sun. ACS Earth and Space Chemistry, 2019, 3, 2110-2121.	1.2	10
39	Destruction of dimethyl ether and methyl formate by collisions with He⁺. Astronomy and Astrophysics, 2019, 625, A72.	2.1	20
40	Molecular Dynamics of CH4/N2 Mixtures on a Flexible Graphene Layer: Adsorption and Selectivity Case Study. Frontiers in Chemistry, 2019, 7, 386.	1.8	14
41	Laboratory Measurements and Astronomical Search for Thioacetamide. ACS Earth and Space Chemistry, 2019, 3, 1537-1549.	1.2	11
42	An Experimental and Theoretical Investigation of 1-Butanol Pyrolysis. Frontiers in Chemistry, 2019, 7, 326.	1.8	12
43	Tuning the magnetic properties of beryllium chains. Physical Chemistry Chemical Physics, 2019, 21, 6080-6086.	1.3	2
44	Interstellar dimethyl ether gas-phase formation: a quantum chemistry and kinetics study. Monthly Notices of the Royal Astronomical Society, 2019, 482, 3567-3575.	1.6	48
45	Combined Experimentalâ€“Theoretical Study of the OH + CO â† H + CO₂ Reaction Dynamics. Journal of Physical Chemistry Letters, 2018, 9, 1229-1236.	2.1	18
46	Possible scenarios for SiS formation in the interstellar medium: Electronic structure calculations of the potential energy surfaces for the reactions of the SiH radical with atomic sulphur and S2. Chemical Physics Letters, 2018, 695, 87-93.	1.2	33
47	A theoretical study on cyclacenes: Analytical tightâ€binding approach. International Journal of Quantum Chemistry, 2018, 118, e25569.	1.0	7
48	Modeling the Interaction of Carbon Monoxide with Flexible Graphene: From Coupled Cluster Calculations to Molecularâ€Dynamics Simulations. ChemPhysChem, 2018, 19, 774-783.	1.0	23
49	The Genealogical Tree of Ethanol: Gas-phase Formation of Glycolaldehyde, Acetic Acid, and Formic Acid. Astrophysical Journal, 2018, 854, 135.	1.6	103
50	Low temperature kinetics and theoretical studies of the reaction CN + CH₃NH₂: a potential source of cyanamide and methyl cyanamide in the interstellar medium. Physical Chemistry Chemical Physics, 2018, 20, 5478-5489.	1.3	33
51	Potential models for the simulation of methane adsorption on graphene: development and CCSD(T) benchmarks. Physical Chemistry Chemical Physics, 2018, 20, 25518-25530.	1.3	23
52	A theoretical investigation of the reaction between the amidogen, NH, and the ethyl, C2H5, radicals: a possible gas-phase formation route of interstellar and planetary ethanimine. Molecular Astrophysics, 2018, 13, 30-37.	1.7	24
53	The evolution of grain mantles and silicate dust growth at high redshift. Monthly Notices of the Royal Astronomical Society, 2018, 476, 1371-1383.	1.6	29
54	A Theoretical Investigation of the Reaction H+SiS2 and Implications for the Chemistry of Silicon in the Interstellar Medium. Lecture Notes in Computer Science, 2018, , 719-729.	1.0	2

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55	Nanostructure Selectivity for Molecular Adsorption and Separation: the Case of Graphyne Layers. Journal of Physical Chemistry C, 2018, 122, 16195-16208.	1.5	32
56	Formation of Nitrogen-Bearing Organic Molecules in the Reaction NHÂ+ÂC2H5: A Theoretical Investigation and Main Implications for Prebiotic Chemistry in Space. Lecture Notes in Computer Science, 2018, , 773-782.	1.0	3
57	Potential Energy Surface for the Interaction of Helium with the Chiral Molecule Propylene Oxide. Lecture Notes in Computer Science, 2018, , 593-604.	1.0	3
58	Confinement of the Pentanitrogen Cation Inside Carbon Nanotubes. Lecture Notes in Computer Science, 2018, , 579-592.	1.0	1
59	Can Formamide Be Formed on Interstellar Ice? An Atomistic Perspective. ACS Earth and Space Chemistry, 2018, 2, 720-734.	1.2	83
60	Nitrogen Gas on Graphene: Pairwise Interaction Potentials. Lecture Notes in Computer Science, 2018, , 563-578.	1.0	3
61	Silicon-bearing molecules in the shock L1157-B1: first detection of SiS around a Sun-like protostar. Monthly Notices of the Royal Astronomical Society: Letters, 2017, 470, L16-L20.	1.2	44
62	Increasing Radical Character of Large [n]cyclacenes Unveiled by Wave Function Theory. Journal of Physical Chemistry A, 2017, 121, 3746-3756.	1.1	45
63	Exploring the Gas Phase Synthesis of the Elusive Class of Boronyls and the Mechanism of Boronyl Radical Reactions under Single Collision Conditions. Accounts of Chemical Research, 2017, 50, 1154-1162.	7.6	16
64	N 3 â^' $_{3}^{-}$ azide anion confined inside finite-size carbon nanotubes. Journal of Molecular Modeling, 2017, 23, 294.	0.8	3
65	Modelization of the $$hbox {H}_{2}$$ H 2 adsorption on graphene and molecular dynamics simulation. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	6
66	Acetone-Water Mixtures: Molecular Dynamics Using a Semiempirical Intermolecular Potential. Lecture Notes in Computer Science, 2017, , 3-13.	1.0	1
67	Molecular Dications in Planetary Atmospheric Escape. Atmosphere, 2016, 7, 112.	1.0	26
68	A Theoretical and Computational Approach to a Semi-classical Model for Electron Spectroscopy Calculations in Collisional Autoionization Processes. Lecture Notes in Computer Science, 2016, , 258-272.	1.0	2
69	A force field for acetone: the transition from small clusters to liquid phase investigated by molecular dynamics simulations. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	19
70	Aqueous N-methylacetamide: New analytic potentials and a molecular dynamics study. Journal of Molecular Liquids, 2016, 224, 792-800.	2.3	15
71	Adsorption of Hydrogen Molecules on Carbon Nanotubes Using Quantum Chemistry and Molecular Dynamics. Journal of Physical Chemistry A, 2016, 120, 6451-6458.	1.1	45
72	Isomer-Specific Chemistry in the Propyne and Allene Reactions with Oxygen Atoms: CH₃CH + CO versus CH₂CH₂ + CO Products. Journal of Physical Chemistry Letters, 2016, 7, 1010-1015.	2.1	23

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73	Collisional Energy Exchange in CO $$_2$$ â€“N $$_2$$ Gaseous Mixtures. Lecture Notes in Computer Science, 2016, , 246-257.	1.0	9
74	A Theoretical Study on the Relevance of Protonated and Ionized Species of Methanimine and Methanol in Astrochemistry. Lecture Notes in Computer Science, 2016, , 296-308.	1.0	1
75	Modeling Combustions: The ab initio Treatment of the O(^{3} P) + CH $$_3$$ OH Reaction. Lecture Notes in Computer Science, 2016, , 71-83.	1.0	0
76	Use of Anticoagulants and Antiplatelet Agents in Stable Outpatients with Coronary Artery Disease and Atrial Fibrillation. International CLARIFY Registry. PLoS ONE, 2015, 10, e0125164.	1.1	15
77	Dimerization of methanimine and its charged species in the atmosphere of Titan and interstellar/cometary ice analogs. Astronomy and Astrophysics, 2015, 584, A76.	2.1	48
78	A combined crossed molecular beam and quasiclassical trajectory study of the Titan-relevant N(2D) + D2O reaction. Molecular Physics, 2015, 113, 2296-2301.	0.8	11
79	CYANOMETHANIMINE ISOMERS IN COLD INTERSTELLAR CLOUDS: INSIGHTS FROM ELECTRONIC STRUCTURE AND KINETIC CALCULATIONS. Astrophysical Journal, 2015, 810, 111.	1.6	53
80	A combined crossed molecular beams and theoretical study of the reaction CN+C2H4. Chemical Physics, 2015, 449, 34-42.	0.9	17
81	Accurate analytic intermolecular potential for the simulation of Na+ and K+ ion hydration in liquid water. Journal of Molecular Liquids, 2015, 204, 192-197.	2.3	42
82	Formation of complex organic molecules in cold objects: the role of gas-phase reactions. Monthly Notices of the Royal Astronomical Society: Letters, 2015, 449, L16-L20.	1.2	218
83	Angular Distributions of Fragment Ions Produced by Coulomb Explosion of Simple Molecular Dications of Astrochemical Interest. Lecture Notes in Computer Science, 2015, , 291-307.	1.0	4
84	A Theoretical Investigation of 1-Butanol Unimolecular Decomposition. Lecture Notes in Computer Science, 2015, , 384-393.	1.0	1
85	Ion-Water Cluster Molecular Dynamics Using a Semiempirical Intermolecular Potential. Lecture Notes in Computer Science, 2015, , 355-370.	1.0	5
86	Energy transfer upon collision of selectively excited CO2 molecules: State-to-state cross sections and probabilities for modeling of atmospheres and gaseous flows. Journal of Chemical Physics, 2015, 143, 034307.	1.2	51
87	Kinetic Energy Release in molecular dications fragmentation after VUV and EUV ionization and escape from planetary atmospheres. Planetary and Space Science, 2014, 99, 149-157.	0.9	49
88	Relevance of the Channel Leading to Formaldehyde + Triplet Ethylidene in the O(³P) + Propene Reaction under Combustion Conditions. Journal of Physical Chemistry Letters, 2014, 5, 4213-4218.	2.1	53
89	Multi-scale theoretical investigation of molecular hydrogen adsorption over graphene: coronene as a case study. RSC Advances, 2014, 4, 54447-54453.	1.7	40
90	Quasiclassical Trajectory Calculations of the N(²D) + H₂O Reaction Elucidating the Formation Mechanism of HNO and HON Seen in Molecular Beam Experiments. Journal of Physical Chemistry Letters, 2014, 5, 3508-3513.	2.1	20

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91	An innovative synergistic grid approach to the computational study of protein aggregation mechanisms. Journal of Molecular Modeling, 2014, 20, 2226.	0.8	32
92	Combined quantum chemical and modeling study of CO hydrogenation on water ice. Astronomy and Astrophysics, 2014, 572, A70.	2.1	87
93	The Escape Probability of Some Ions from Mars and Titan Ionospheres. Lecture Notes in Computer Science, 2014, , 554-570.	1.0	9
94	The Molecular Stirrer Catalytic Effect in Methane Ice Formation. Lecture Notes in Computer Science, 2014, , 585-600.	1.0	16
95	Grid Calculation Tools for Massive Applications of Collision Dynamics Simulations: Carbon Dioxide Energy Transfer. Lecture Notes in Computer Science, 2014, , 627-639.	1.0	6
96	Production of ions at high energy and its role in extraterrestrial environments. Rendiconti Lincei, 2013, 24, 53-65.	1.0	45
97	A Theoretical Study of Formation Routes and Dimerization of Methanimine and Implications for the Aerosols Formation in the Upper Atmosphere of Titan. Lecture Notes in Computer Science, 2013, , 47-56.	1.0	16
98	A highâ€level ab initio study of the N₂ + N₂ reaction channel. Journal of Computational Chemistry, 2013, 34, 2668-2676.	1.5	44
99	Modeling of Energy Transfer From Vibrationally Excited CO₂ Molecules: Cross Sections and Probabilities for Kinetic Modeling of Atmospheres, Flows, and Plasmas. Journal of Physical Chemistry A, 2013, 117, 11430-11440.	1.1	43
100	Competitive solvation of K+ by C6H6 and H2O in the K+-(C6H6)n-(H2O)m (nÂ=Â1â€“4; mÂ=Â1â€“6) aggregates. European Physical Journal D, 2013, 67, 1.	0.6	35
101	Design and implementation of a Grid application for direct calculations of reactive rates. Computational and Theoretical Chemistry, 2013, 1022, 103-107.	1.1	10
102	Combined crossed beam and theoretical studies of the C(1D) + CH4 reaction. Journal of Chemical Physics, 2013, 138, 024311.	1.2	40
103	Water (H2O) m or Benzene (C6H6) n Aggregates to Solvate the Kâ€‰+â€‰?. Lecture Notes in Computer Science, 2013, , 1-15.	1.0	23
104	Modeling the Intermolecular Interactions and Characterization of the Dynamics of Collisional Autoionization Processes. Lecture Notes in Computer Science, 2013, , 69-83.	1.0	33
105	Carbon Oxides in Gas Flows and Earth and Planetary Atmospheres: State-to-State Simulations of Energy Transfer and Dissociation Reactions. Lecture Notes in Computer Science, 2013, , 17-31.	1.0	26
106	Ion Size Influence on the Ar Solvation Shells of M⁺â€“C₆F₆ Clusters (M = Na, K, Rb, Cs). Journal of Physical Chemistry A, 2012, 116, 3094-3102.	1.1	35
107	Combined Crossed Beam and Theoretical Studies of the N(²D) + C₂H₄Reaction and Implications for Atmospheric Models of Titan. Journal of Physical Chemistry A, 2012, 116, 10467-10479.	1.1	58
108	Crossed molecular beam studies of bimolecular reactions of relevance in combustion. Energy, 2012, 43, 47-54.	4.5	25

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109	Biogas steam and oxidative reforming processes for synthesis gas and hydrogen production in conventional and microreactor reaction systems. International Journal of Hydrogen Energy, 2012, 37, 13829-13842.	3.8	64
110	Collisional autoionization dynamics of Neâˆ—(3P2,0)â€“H2O. Chemical Physics Letters, 2012, 546, 34-39.	1.2	38
111	The last mile of molecular reaction dynamics virtual experiments: the case of the OH(N = 1â€“10) + CO(j =) Tj ETQq1 1 0.784314 rgB	1.6	28
112	Elementary reactions of N atoms with hydrocarbons: first steps towards the formation of prebiotic N-containing molecules in planetary atmospheres. Chemical Society Reviews, 2012, 41, 5473.	18.7	67
113	Benzene water interaction: From gaseous dimers to solvated aggregates. Chemical Physics, 2012, 399, 232-239.	0.9	46
114	An extension of the grid empowered molecular simulator to quantum reactive scattering. Journal of Computational Chemistry, 2012, 33, 708-714.	1.5	26
115	Theoretical Study of Reactions Relevant for Atmospheric Models of Titan: Interaction of Excited Nitrogen Atoms with Small Hydrocarbons. Lecture Notes in Computer Science, 2012, , 331-344.	1.0	19
116	A Bond-Bond Portable Approach to Intermolecular Interactions: Simulations for N-methylacetamide and Carbon Dioxide Dimers. Lecture Notes in Computer Science, 2012, , 387-400.	1.0	34
117	Crossed-beam dynamics studies of the radicalâ€“radical combustion reaction O(³P) + CH₃(methyl). Physical Chemistry Chemical Physics, 2011, 13, 8322-8330.	1.3	19
118	Low temperature kinetics, crossed beam dynamics and theoretical studies of the reaction S(1D) + CH4 and low temperature kinetics of S(1D) + C2H2. Physical Chemistry Chemical Physics, 2011, 13, 8485.	1.3	31
119	Ar Solvation Shells in K⁺â€“HFBz: From Cluster Rearrangement to Solvation Dynamics. Journal of Physical Chemistry A, 2011, 115, 10871-10879.	1.1	28
120	A portable intermolecular potential for molecular dynamics studies of NMAâ€“NMA and NMAâ€“H2O aggregates. Physical Chemistry Chemical Physics, 2011, 13, 8422.	1.3	43
121	Crossed molecular beam studies of astronomically relevant bimolecular reactions. Rendiconti Lincei, 2011, 22, 173-181.	1.0	4
122	An Extension of the Molecular Simulator GEMS to Calculate the Signal of Crossed Beam Experiments. Lecture Notes in Computer Science, 2011, , 453-465.	1.0	14
123	COMPCHEM: Progress Towards GEMS a Grid Empowered Molecular Simulator and Beyond. Journal of Grid Computing, 2010, 8, 571-586.	2.5	63
124	Direct calculation of the rate coefficients on the grid: Exact quantum versus semiclassical results for N + N₂. International Journal of Quantum Chemistry, 2010, 110, 422-431.	1.0	8
125	Formation of nitriles and imines in the atmosphere of Titan: combined crossed-beam and theoretical studies on the reaction dynamics of excited nitrogen atoms N(2D) with ethane. Faraday Discussions, 2010, 147, 189.	1.6	79
126	Distributed and Collaborative Learning Objects Repositories on Grid Networks. Lecture Notes in Computer Science, 2010, , 29-40.	1.0	15

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127	Elementary Reactions and Their Role in Gas-Phase Prebiotic Chemistry. International Journal of Molecular Sciences, 2009, 10, 2304-2335.	1.8	92
128	On the suitability of the ILJ function to match different formulations of the electrostatic potential for water-water interactions. European Physical Journal D, 2009, 55, 75-85.	0.6	75
129	Combined Crossed Molecular Beam and Theoretical Studies of the N(²D) + CH₄ Reaction and Implications for Atmospheric Models of Titan. Journal of Physical Chemistry A, 2009, 113, 11138-11152.	1.1	90
130	Tetrahedral Ordering in Water: Raman Profiles and Their Temperature Dependence. Journal of Physical Chemistry A, 2009, 113, 15100-15105.	1.1	66
131	Observation of organosulfur products (thiovinoxy, thioketene and thioformyl) in crossed-beam experiments and low temperature rate coefficients for the reaction S(1D) + C2H4. Physical Chemistry Chemical Physics, 2009, 11, 4701.	1.3	33
132	Crossed-Beam Dynamics, Low-Temperature Kinetics, and Theoretical Studies of the Reaction S(¹D) + C₂H₄. Journal of Physical Chemistry A, 2009, 113, 15328-15345.	1.1	38
133	Crossed-Beam and Theoretical Studies of the S(¹D) + C₂H₂ Reaction. Journal of Physical Chemistry A, 2009, 113, 4330-4339.	1.1	28
134	A Grid Implementation of Direct Semiclassical Calculations of Rate Coefficients. Lecture Notes in Computer Science, 2009, , 93-103.	1.0	3
135	A Grid Implementation of Direct Quantum Calculations of Rate Coefficients. Lecture Notes in Computer Science, 2009, , 104-114.	1.0	1
136	Full dimensional quantum versus semiclassical reactivity for the bent transition state reaction N+N2. Chemical Physics Letters, 2008, 464, 249-255.	1.2	20
137	Thermal rate coefficients in collinear versus bent transition state reactions: the N+N₂case study. Physica Scripta, 2008, 78, 058116.	1.2	25
138	Toward a Fuzzy Astrophysics Research Resources (FARR). , 2007, , .		0
139	Quantum vs Semiclassical Dynamics Approaches from highly symmetric to asymmetric reactions. , 2007, , .		1
140	Structural Order in Water: Comparison between the Spectral Analysis of Raman Data and Molecular Dynamics Results. AIP Conference Proceedings, 2007, , .	0.3	0
141	On the semiclassical initial value calculation of thermal rate coefficients for the N+N2 reaction. Journal of Chemical Physics, 2006, 125, 114311.	1.2	24
142	A Simplified Myoglobin Model for Molecular Dynamics Calculations. Lecture Notes in Computer Science, 2006, , 731-737.	1.0	0
143	A comparison of semiclassical IVR and exact quantum collinear atom diatom transition probabilities for mixed reactive and non reactive regimes. AIP Conference Proceedings, 2005, , .	0.3	7
144	Dynamics of the O(3P) + C2H4Reaction:Â Identification of Five Primary Product Channels (Vinoxy, Acetyl,) Tj ETQq0 0 0 rgBT /Overlock 1 Soft Electron Ionization. Journal of Physical Chemistry A, 2005, 109, 3527-3530.	1.1	74

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145	Thermal Rate Coefficients for the N + N 2 Reaction: Quasiclassical, Semiclassical and Quantum Calculations. Lecture Notes in Computer Science, 2005, , 1083-1092.	1.0	4
146	Quantum vs. semiclassic initial value representation probabilities for nonreactive systems. International Journal of Quantum Chemistry, 2004, 96, 547-553.	1.0	2
147	A Nonorthogonal Coordinate Approach to Atom-Diatom Parallel Reactive Scattering Calculations. Collection of Czechoslovak Chemical Communications, 2003, 68, 307-330.	1.0	22
148	Initial Value Semiclassical Approaches to Reactive and Non Reactive Transition Probabilities. Lecture Notes in Computer Science, 2003, , 357-365.	1.0	0
149	Observation of Nitrogen-Bearing Organic Molecules from Reactions of Nitrogen Atoms with Hydrocarbons:â€‰ A Crossed Beam Study of N(2D) + Ethylene. Journal of Physical Chemistry A, 2000, 104, 5655-5659.	1.1	70