Antonio Lagana

List of Publications by Year
in descending order

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165	2,276	236833	345118
papers	citations	25 h-index	36 g-index

174	174	174	709
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Methane Production from H2 + CO2 Reaction: An Open Molecular Science Case for Computational and Experimental Studies. Physchem, 2021, 1, 82-94.	0.5	1
2	Free-Methane - from the Ionosphere of Mars Towards a Prototype Methanation Reactor: A Project Producing Fuels via Plasma Assisted Carbon Dioxide Hydrogenation. Lecture Notes in Computer Science, 2021, , 594-607.	1.0	0
3	Collisional O2 + N2 State-Selected Cross Sections for Open Science Cloud Reuse. Journal of Physical Chemistry A, 2020, 124, 6445-6457.	1.1	2
4	Kinetics Of The H + CH₂ â†' CH + H₂ Reaction At Low Temperature. Journal of Physical Chemistry A, 2019, 123, 7408-7419.	1.1	5
5	Cloud and Local Servers for a Federation of Molecular Science Learning Object Repositories. Lecture Notes in Computer Science, 2019, , 359-373.	1.0	5
6	The ECTN Virtual Education Community Prosumer Model for Promoting and Assessing Chemical Knowledge. Lecture Notes in Computer Science, 2018, , 533-548.	1.0	12
7	Sharing Learning Objects Between Learning Platforms and Repositories. Lecture Notes in Computer Science, 2018, , 804-816.	1.0	2
8	A quantum-classical study of the OH + H 2 reactive and inelastic collisions. Chemical Physics Letters, 2017, 674, 103-108.	1.2	8
9	Comparisons and scaling rules between N+N₂and N₂+N₂collision induced dissociation cross sections from atomistic studies. Plasma Sources Science and Technology, 2017, 26, 045005.	1.3	17
10	The role of the long-range tail of the potential in O₂ + N₂ collisional inelastic vibrational energy transfers. Physical Chemistry Chemical Physics, 2017, 19, 11206-11211.	1.3	10
11	Methane production by CO2 hydrogenation reaction with and without solid phase catalysis. Fuel, 2017, 209, 802-811.	3.4	25
12	A Dynamics Investigation of the C + CH⁺â†' C₂⁺+ H Reaction on an ab Initio Bond-Order-Like Potential. Journal of Physical Chemistry A, 2016, 120, 5125-5135.	1.1	15
13	Autobiography of Antonio LaganÃ: Toward the Design of a European Integrated Collaborative Distributed Research Infrastructure for the Study of Molecular Processes. Journal of Physical Chemistry A, 2016, 120, 4589-4594.	1.1	1
14	Energy transfer dynamics and kinetics of elementary processes (promoted) by gasâ€phase CO₂â€N₂ collisions: Selectivity control by the anisotropy of the interaction. Journal of Computational Chemistry, 2016, 37, 1463-1475.	1.5	36
15	Simulation of Methane Production from Carbon Dioxide on a Collaborative Research Infrastructure. Lecture Notes in Computer Science, 2016, , 319-333.	1.0	1
16	Mobile Device Access to Collaborative Distributed Repositories of Chemistry Learning Objects. Lecture Notes in Computer Science, 2016, , 443-454.	1.0	5
17	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
18	Quasi-resonant vibrational energy transfer in N2+N2 collisions: Effect of the long-range interaction. Chemical Physics Letters, 2015, 620, 103-108.	1.2	20

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19	Exchange of Learning Objects Between a Learning Management System and a Federation of Science Distributed Repositories. Lecture Notes in Computer Science, 2015, , 371-383.	1.0	7
20	Ion-Water Cluster Molecular Dynamics Using a Semiempirical Intermolecular Potential. Lecture Notes in Computer Science, 2015, , 355-370.	1.0	5
21	Code interoperability and standard data formats in quantum chemistry and quantum dynamics: The Q5/D5Cost data model. Journal of Computational Chemistry, 2014, 35, 611-621.	1.5	22
22	The effect of the intermolecular potential formulation on the stateâ€selected energy exchange rate coefficients in N₂â€“N₂ collisions. Journal of Computational Chemistry, 2014, 35, 722-736.	1.5	17
23	An innovative synergistic grid approach to the computational study of protein aggregation mechanisms. Journal of Molecular Modeling, 2014, 20, 2226.	0.8	32
24	Learning Objects Efficient Handling in a Federation of Science Distributed Repositories. Lecture Notes in Computer Science, 2014, , 615-626.	1.0	14
25	Electronuclear multiconfiguration timeâ€dependent hartree calculations on the confined H atom with mobile electron and nucleus. International Journal of Quantum Chemistry, 2013, 113, 1333-1338.	1.0	3
26	An approximate quantum mechanical study of the N+Oâ†'NO++eâ^' associative ionisation. Chemical Physics Letters, 2013, 557, 43-48.	1.2	3
27	Quantum reactive scattering on innovative computing platforms. Computer Physics Communications, 2013, 184, 1372-1380.	3.0	7
28	MCTDH calculations on the rigid OH radical moving along a (10,0) carbon nanotube. Chemical Physics Letters, 2013, 575, 18-22.	1.2	16
29	Cooperative modelling and design on the computing grid: data, flux and knowledge interoperability. Journal of Molecular Modeling, 2013, 19, 4215-4222.	0.8	1
30	An Efficient Taxonomy Assistant for a Federation of Science Distributed Repositories: A Chemistry Use Case. Lecture Notes in Computer Science, 2013, , 96-109.	1.0	10
31	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
32	An innovative computational comparison of exact and centrifugal sudden quantum properties of the N + N₂reaction. Physical Chemistry Chemical Physics, 2012, 14, 1589-1595.	1.3	4
33	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
34	A molecular dynamics study of sodium dodecyl sulfateâ€methane system in water using the improved lennard jones formulation. International Journal of Quantum Chemistry, 2012, 112, 1810-1817.	1.0	6
35	A full dimensional grid empowered simulation of the CO₂ + CO₂ processes. Journal of Computational Chemistry, 2012, 33, 1806-1819.	1.5	69
36	An extension of the grid empowered molecular simulator to quantum reactive scattering. Journal of Computational Chemistry, 2012, 33, 708-714.	1.5	26

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37	Quantum Reactive Scattering Calculations on GPU. Lecture Notes in Computer Science, 2012, , 292-303.	1.0	3
38	Efficient Workload Distribution Bridging HTC and HPC in Scientific Computing. Lecture Notes in Computer Science, 2012, , 345-357.	1.0	6
39	Taxonomy Management in a Federation of Distributed Repositories: A Chemistry Use Case. Lecture Notes in Computer Science, 2012, , 358-370.	1.0	15
40	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
41	A Grid Execution Model for Computational Chemistry Applications Using the GC3Pie Framework and the AppPot VM Environment. Lecture Notes in Computer Science, 2012, , 401-416.	1.0	3
42	The MPI Structure of Chimere. Lecture Notes in Computer Science, 2012, , 417-431.	1.0	0
43	Time Dependent Quantum Reactive Scattering on GPU. Lecture Notes in Computer Science, 2011, , 428-441.	1.0	4
44	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
45	Federation of Distributed and Collaborative Repositories and Its Application on Science Learning Objects. Lecture Notes in Computer Science, 2011, , 466-478.	1.0	16
46	On the extension of the grid-empowered molecular science simulator: MD and visualisation tools. International Journal of Web and Grid Services, 2010, 6, 141.	0.4	5
47	A study of the impact of long range interactions on the reactivity of N + N<SUB align=right>2 using the Grid Empowered Molecular Simulator GEMS. International Journal of Web and Grid Services, 2010, 6, 196.	0.4	11
48	COMPCHEM: Progress Towards GEMS a Grid Empowered Molecular Simulator and Beyond. Journal of Grid Computing, 2010, 8, 571-586.	2.5	63
49	Anionâ€Dependent Tendency of Diâ€Longâ€Chain Quaternary Ammonium Salts to Form Ion Quadruples and Higher Aggregates in Benzene. ChemPhysChem, 2010, 11, 3243-3254.	1.0	36
50	Non-Bornâ€“Oppenheimer MCTDH calculations on the confined H2+ molecular ion. Chemical Physics Letters, 2010, 500, 144-148.	1.2	11
51	Microscopic branching processes: The O + O₂ reaction and its relaxed potential representations. International Journal of Quantum Chemistry, 2010, 110, 358-367.	1.0	21
52	A priori molecular virtual reality on EGEE grid. International Journal of Quantum Chemistry, 2010, 110, 446-453.	1.0	8
53	Porting of GROMACS Package into the Grid Environment: Testing of a New Distribution Strategy. Lecture Notes in Computer Science, 2010, , 41-52.	1.0	3
54	Effect of the Total Angular Momentum on the Dynamics of the H₂ + H₂ System. Journal of Physical Chemistry A, 2009, 113, 14312-14320.	1.1	7

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55	Apparent conflicting indications on the conformation of dimethyletherâ€“argon from the rotational spectra of the d6 and 13C species. Journal of Molecular Spectroscopy, 2009, 257, 29-33.	0.4	3
56	The O + O2 reaction: quantum detailed probabilities and thermal rate coefficients. Theoretical Chemistry Accounts, 2009, 123, 249-256.	0.5	19
57	A program for performing exact quantum dynamics calculations using cylindrical polar coordinates: A nanotube application. Computer Physics Communications, 2009, 180, 459-465.	3.0	5
58	A detailed comparison of centrifugal sudden and J-shift estimates of the reactive properties of the N + N2 reaction. Physical Chemistry Chemical Physics, 2009, 11, 11456.	1.3	10
59	A comparison of the quantum state-specific efficiency of N + N2 reaction computed on different potential energy surfaces. Physical Chemistry Chemical Physics, 2009, 11, 1752.	1.3	30
60	A Grid Implementation of Chimere: Ozone Production in Central Italy. Lecture Notes in Computer Science, 2009, , 115-129.	1.0	1
61	A Grid Implementation of Direct Semiclassical Calculations of Rate Coefficients. Lecture Notes in Computer Science, 2009, , 93-103.	1.0	3
62	A Grid Implementation of Direct Quantum Calculations of Rate Coefficients. Lecture Notes in Computer Science, 2009, , 104-114.	1.0	1
63	Correlation of attack and recoil angles for the Li+HF reaction: An exact quantum mechanical study at low and high total angular momentum. Chemical Physics, 2008, 349, 170-180.	0.9	13
64	Full dimensional quantum versus semiclassical reactivity for the bent transition state reaction N+N2. Chemical Physics Letters, 2008, 464, 249-255.	1.2	20
65	Implementation of the ABC Quantum Mechanical Reactive Scattering Program on the EGEE Grid Platform. Lecture Notes in Computer Science, 2008, , 1108-1120.	1.0	5
66	Modeling the global potential energy surface of the N + N2 reaction from ab initio data. Physical Chemistry Chemical Physics, 2008, 10, 2552.	1.3	39
67	Thermal rate coefficients in collinear versus bent transition state reactions: the N+N₂case study. Physica Scripta, 2008, 78, 058116.	1.2	25
68	Investigation of Propane and Methane Bulk Properties Structure Using Two Different Force Fields. Lecture Notes in Computer Science, 2008, , 1052-1064.	1.0	5
69	FITTING: A Portal to Fit Potential Energy Functionals to ab initio Points. Lecture Notes in Computer Science, 2007, , 358-365.	1.0	0
70	An alternative distribution model for the Molecular Dynamics study of liquid Propane on a grid platform. , 2007, , .		1
71	Quantum mechanical study of the correlation of attack and recoil angles for the Li+HF reaction: Stereodirected versus discrete variable representations. Chemical Physics Letters, 2007, 440, 1-6.	1.2	12
72	A detailed trajectory study of the OH+COâ†'H+CO2 reaction. Chemical Physics, 2007, 332, 162-175.	0.9	21

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73	Quantum dynamics of H atom transmission across carbon nanotubes. Theoretical Chemistry Accounts, 2007, 118, 47-52.	0.5	6
74	Quantum Mechanical Study of the Correlation of Attack and Recoil Angles for the Cl + H2Reaction Using the Stereodirected and Discrete Variable Representations on Two Potential Energy Surfacesâ€. Journal of Physical Chemistry A, 2006, 110, 5289-5294.	1.1	4
75	On the Structuring of the Computational Chemistry Virtual Organization COMPCHEM. Lecture Notes in Computer Science, 2006, , 665-674.	1.0	50
76	Calculated versus measured product distributions of the OH+D 2 reaction. Molecular Physics, 2006, 104, 839-846.	0.8	9
77	EChemTest: The Assessment of Chemistry Knowledge. Nachrichten Aus Der Chemie, 2006, 54, 1272-1272.	0.0	1
78	Immersive Molecular Virtual Reality Based on X3D and Web Services. Lecture Notes in Computer Science, 2006, , 212-221.	1.0	7
79	Atom-Bond Additive Potentials for Benzene-Rare Gas Clusters. Lecture Notes in Computer Science, 2006, , 721-730.	1.0	2
80	A multiproperty analysis of the OH+H2(D2,HD) potential energy surface. Chemical Physics, 2005, 308, 201-210.	0.9	7
81	A Molecular Dynamics Study of Ion Permeability Through Molecular Pores. Lecture Notes in Computer Science, 2005, , 1093-1100.	1.0	7
82	A Grid Molecular Simulator for E-Science. Lecture Notes in Computer Science, 2005, , 16-22.	1.0	11
83	Virtual Chemical Laboratories and Their Management on the Web. Lecture Notes in Computer Science, 2005, , 905-912.	1.0	5
84	Ab Initio and Empirical Atom Bond Formulation of the Interaction of the Dimethylether-Ar System. Lecture Notes in Computer Science, 2005, , 1046-1053.	1.0	6
85	Integrating Learning and Assessment Using the Semantic Web. Lecture Notes in Computer Science, 2005, , 921-927.	1.0	4
86	Virtual Reality Applied to Molecular Sciences. Lecture Notes in Computer Science, 2004, , 827-836.	1.0	6
87	EoL: A Web-Based Distance Assessment System. Lecture Notes in Computer Science, 2004, , 854-862.	1.0	6
88	Bond Order Potentials for a priori Simulations of Polyatomic Reactions. Lecture Notes in Computer Science, 2004, , 328-337.	1.0	3
89	A Time Dependent Study of the Nitrogen Atom Nitrogen Molecule Reaction. Lecture Notes in Computer Science, 2004, , 357-365.	1.0	6
90	Time-dependent wavepacket calculations for the system on a LEPS surface: inelastic and reactive probabilities. Molecular Physics, 2004, 102, 2237-2248.	0.8	22

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91	Wave packet calculations for the Cl + H2reaction. International Journal of Quantum Chemistry, 2004, 96, 562-567.	1.0	29
92	Rotational and alignment effects in a wave packet calculation for the Cl + H2reaction. International Journal of Quantum Chemistry, 2004, 99, 577-584.	1.0	18
93	Rotational and alignment effects in a multisurface wavepacket calculation for the Cl + H2reaction. Physical Chemistry Chemical Physics, 2004, 6, 5000-5006.	1.3	13
94	A Full Dimensional Quasiclassical Trajectory Study of Cl + CH4Rate Coefficientsâ€. Journal of Physical Chemistry A, 2004, 108, 8752-8758.	1.1	15
95	Towards a Grid Based Universal Molecular Simulator. , 2004, , 363-380.		5
96	Fine Grain Parallelization of a Discrete Variable Wavepacket Calculation Using ASSIST-CL. Lecture Notes in Computer Science, 2004, , 437-444.	1.0	1
97	Isotopic effects in the product vibrational distribution of the OH(OD)+HCl reaction. Chemical Physics Letters, 2003, 371, 223-228.	1.2	10
98	A LAGROBO Multiproperty Fit to Four-Atom Potential Energy Surfaces:â€‰ The OH + HCl Case Study. Journal of Physical Chemistry A, 2003, 107, 7248-7257.	1.1	9
99	Linear Algebra Computation Benchmarks on a Model Grid Platform. Lecture Notes in Computer Science, 2003, , 297-306.	1.0	8
100	A Multiscale Virtual Reality Approach to Chemical Experiments. Lecture Notes in Computer Science, 2003, , 324-330.	1.0	9
101	A Nonorthogonal Coordinate Approach to Atom-Diatom Parallel Reactive Scattering Calculations. Collection of Czechoslovak Chemical Communications, 2003, 68, 307-330.	1.0	22
102	Reaction and dissociation mechanism control: the H2â€‰+â€‰H2system. Physical Chemistry Chemical Physics, 2002, 4, 5007-5013.	1.3	9
103	A prototype of a Problem Solving Environment for an a priori Molecular Simulator on the Grid. Journal of Computational Methods in Sciences and Engineering, 2002, 2, 377-383.	0.1	1
104	Ab initio calculation and quasi-classical dynamics study of the two lowest potential energy surfaces of the O(1D)+HBr system*. International Journal of Quantum Chemistry, 2002, 86, 79-89.	1.0	8
105	A LAGROBO strategy to fit potential energy surfaces: the OH+HCl reaction. Chemical Physics Letters, 2002, 360, 304-312.	1.2	27
106	Towards a GRID based Portal for an a priori Molecular Simulation of Chemical Reactivity. Lecture Notes in Computer Science, 2002, , 956-965.	1.0	13
107	Parallel Approaches to the Integration of the Differential Equations for Reactive Scattering. Lecture Notes in Computer Science, 2002, , 908-917.	1.0	1
108	Fine Grain Parallelism for Discrete Variable Approaches to Wavepacket Calculations. Lecture Notes in Computer Science, 2002, , 918-925.	1.0	6

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109	Parallel skeletons and computational grain in quantum reactive scattering calculations. , 2002, , .		2
110	State and orientation selected reactivity of O(1D) + HCl from wavepacket calculations Presented at the Stereodynamics 2000 Conference on Dynamics and Stereodynamics of Chemical Reactions, El Escorial, Madrid, December 1Ã¢â‚¬â€œ5, 2000.. Physical Chemistry Chemical Physics, 2001, 3, 4515-4521.	1.3	22
111	Wave Packet Calculation of Cross Sections, Product State Distributions, and Branching Ratios for the O(1D) + HCl Reaction. Journal of Physical Chemistry A, 2001, 105, 5743-5750.	1.1	30
112	Li + HF:Â A Case Study to Develop Novel Computational Technologies for Reactive Scatteringâ€. Journal of Physical Chemistry A, 2001, 105, 2361-2368.	1.1	3
113	Progress in validating the potential energy surface of the OH+H2 reaction: product vibrational distributions. Chemical Physics Letters, 2001, 345, 219-227.	1.2	12
114	On the effect of increasing the total angular momentum on Li+HF reactivity. Chemical Physics Letters, 2000, 324, 466-474.	1.2	25
115	Computational granularity and parallel models to scale up reactive scattering calculations. Computer Physics Communications, 2000, 128, 295-314.	3.0	8
116	Quantum isotopic effects and reaction mechanisms: the Li+HF reaction. Physical Chemistry Chemical Physics, 2000, 2, 535-540.	1.3	22
117	Quasiclassical trajectory simulation of the O(1D)+HClâ†'OH+Cl, ClO+H reactions on an improved potential energy surface. Physical Chemistry Chemical Physics, 2000, 2, 589-597.	1.3	46
118	A Web-Based Metacomputing Problem-Solving Environment for Complex Applications. Lecture Notes in Computer Science, 2000, , 111-122.	1.0	7
119	Time Independent 3D Quantum Reactive Scattering on MIMD Parallel Computers. Lecture Notes in Computer Science, 2000, , 338-345.	1.0	1
120	On the Optimization of a Pipeline Model to Integrate a Reduced-Dimensionality SchrÃ¶dinger Equation for Distributed Memory Architectures. International Journal of High Performance Computing Applications, 1999, 13, 49-62.	2.4	2
121	Innovative computing and detailed properties of elementary reactions using time independent approaches. Computer Physics Communications, 1999, 116, 1-16.	3.0	36
122	The influence of initial energy on product vibrational distributions and isotopic mass effects in endoergic reactions: the Mg+FH case. Physical Chemistry Chemical Physics, 1999, 1, 1133-1139.	1.3	2
123	Attack and Recoil Angle Dependence of the Li + HF â†' LiF + H Reaction atJ= 0. Journal of Physical Chemistry A, 1999, 103, 10776-10782.	1.1	17
124	Energy mode effectiveness and tunnelling in triatomic reactions: the energy threshold for the Mg+FHâ†'MgF+H reaction. Chemical Physics Letters, 1998, 282, 91-99.	1.2	6
125	Rate coefficients under jet conditions. Plasma Sources Science and Technology, 1998, 7, 359-362.	1.3	5
126	Parallel quantum scattering calculations applied to the dynamics of elementary reactions. Lecture Notes in Computer Science, 1998, , 331-337.	1.0	6

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127	A model for parallel one dimensional eigenvalues and eigenfunctions calculations. Lecture Notes in Computer Science, 1998, , 364-370.	1.0	1
128	Ab initio calculations and dynamical tests of a potential energy surface for the Na+FH reaction. Journal of Chemical Physics, 1997, 106, 10222-10229.	1.2	27
129	Eigensolutions for one-dimensional cuts of bond order potentials. Chemical Physics Letters, 1997, 267, 403-410.	1.2	5
130	Anabinitiostudy of the O(1D)+HCl reaction. Journal of Chemical Physics, 1996, 105, 2710-2718.	1.2	50
131	Recoil opacity function and angular momentum transfer across a deep well for heavy heavy-light chemical reactions. Chemical Physics Letters, 1995, 241, 408-414.	1.2	5
132	Distributed computing for quantum reactive scattering calculations. AIP Conference Proceedings, 1995, , .	0.3	1
133	Threshold Effects and Reaction Barrier in the Li + FH Reaction and Its Isotopic Variants. The Journal of Physical Chemistry, 1995, 99, 11696-11700.	2.9	18
134	From parallel to distributed computing for reactive scattering calculations. International Journal of Quantum Chemistry, 1994, 52, 85-102.	1.0	6
135	Temperature dependence of nitrogen atom-molecule rate coefficients. The Journal of Physical Chemistry, 1994, 98, 502-507.	2.9	100
136	Cooperative mechanisms for the Hâ€,+â€,ICl reaction and their significance for the Kâ€,+â€,ICl experiment. Canadian Journal of Chemistry, 1994, 72, 919-927.	0.6	3
137	The potential energy surface of the Na(32S12)+HF(X1Î£+) reaction. Chemical Physics Letters, 1993, 202, 284-290.	1.2	18
138	Where are embarrassingly parallel problems? The atom-diatom quasiclassical reactivity. Theoretica Chimica Acta, 1993, 84, 413-421.	0.9	10
139	Calculated versus measured vibrational state specific reactivity of hydrogen atom + fluorine. The Journal of Physical Chemistry, 1993, 97, 8578-8582.	2.9	20
140	The ridge of the specific opacity surface in heavy heavyâ€“light chemical reactions. Journal of Chemical Physics, 1993, 98, 5102-5103.	1.2	2
141	A comparison of timeâ€dependent and timeâ€independent quantum reactive scatteringâ€”Li+HFâ†’LiF+H model calculations. Journal of Chemical Physics, 1993, 99, 9567-9584.	1.2	63
142	Molecular-like behavior and vector correlations for the magnesium + hydrogen fluoride reaction. The Journal of Physical Chemistry, 1992, 96, 3587-3590.	2.9	14
143	Potential energy representations in the bond order space. Chemical Physics, 1992, 168, 341-348.	0.9	30
144	The impact of parallel computing on reactive scattering calculations. Computer Physics Communications, 1992, 70, 223-241.	3.0	5

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145	Heavyâ€"heavyâ€"light limit and exchanged-atom isotopic effects in atomâ€"diatom reactivity. Chemical Physics Letters, 1992, 189, 138-143.	1.2	10
146	A rotating bond order formulation of the atom diatom potential energy surface. Journal of Chemical Physics, 1991, 95, 2216-2217.	1.2	52
147	Reactive Collisional Spectroscopy: Scalar and Vector Information From Numerically Intensive Computing. Laser Chemistry, 1991, 11, 169-175.	0.5	0
148	Scalar and vector properties of the magnesium + hydrogen fluoride reaction on a bond order surface. The Journal of Physical Chemistry, 1991, 95, 8379-8384.	2.9	24
149	Parallel calculations of quasiclassical rate constants: the H + H2 reaction. Chemical Physics Letters, 1991, 176, 273-279.	1.2	6
150	Parallel calculations of approximate 3D quantum cross sections: the Li + HF reaction. Chemical Physics Letters, 1991, 176, 280-286.	1.2	18
151	Li + HCl RIOSA cross section calculations on parallel computers. Theoretica Chimica Acta, 1991, 79, 191-198.	0.9	13
152	D+D 2 Quasiclassical rate constant calculations on parallel computers. Theoretica Chimica Acta, 1991, 79, 323-333.	0.9	8
153	Twoâ€vector correlations and microscopic branching in chemical dynamics: Alignment and orientation effects for the Mg+HFâ†'MgF+H reaction. Journal of Chemical Physics, 1991, 95, 998-1005.	1.2	22
154	About the convergence of reactive infinite order sudden calculations on parallel computers. Journal of Chemical Physics, 1991, 95, 2218-2219.	1.2	9
155	Macroscopic indicators for microscopic branching: The Be+HFâ†'BeF+H chemical reaction. Chemical Physics Letters, 1990, 168, 448-453.	1.2	6
156	Competing mechanisms and productsâ€™ properties for the Be+HF reaction. Journal of Chemical Physics, 1990, 93, 1082-1088.	1.2	4
157	On the all channels representation of the potential energy surface for reactive collisions. Chemical Physics Letters, 1989, 158, 87-94.	1.2	15
158	An approximate three-dimensional quantum-mechanical study of the Li+HFâ†'LiF+H reaction. Chemical Physics Letters, 1989, 158, 362-368.	1.2	14
159	A potential energy surface for the Li+HCl reaction. Journal of Chemical Physics, 1988, 88, 181-190.	1.2	30
160	Vibrational deactivation mechanisms for O+2(v=1) colliding with Kr. Journal of Chemical Physics, 1988, 88, 4814-4818.	1.2	23
161	On the Franckâ€"Condon behavior of the H+Cl2reaction. Journal of Chemical Physics, 1987, 86, 5523-5533.	1.2	11
162	An approximate estimate of the Li+HF reactivity. Chemical Physics Letters, 1987, 139, 140-144.	1.2	13

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163	Computational evidence for the existence of two mechanisms for the vibrational relaxation of O+2 by collision with Kr. Chemical Physics Letters, 1987, 136, 398-401.	1.2	17
164	Two-configuration mc potential energy surface for the reaction of Mg with HF. Chemical Physics, 1986, 101, 55-65.	0.9	14
165	Two-configuration potential energy surface for the collinear Ca + HF â†' CaF + H reaction. Chemical Physics Letters, 1986, 126, 330-334.	1.2	13