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	Temperature dependence of nitrogen atom-molecule rate coefficients. The Journal of Physical Chemistry, 1994, 98, 502-507.	2.9	100
2	A full dimensional grid empowered simulation of the CO₂ + CO₂ processes. Journal of Computational Chemistry, 2012, 33, 1806-1819.	1.5	69
3	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
4	COMPCHEM: Progress Towards GEMS a Grid Empowered Molecular Simulator and Beyond. Journal of Grid Computing, 2010, 8, 571-586.	2.5	63
5	A rotating bond order formulation of the atom diatom potential energy surface. Journal of Chemical Physics, 1991, 95, 2216-2217.	1.2	52
6	Anabinitiostudy of the O(1D)+HCl reaction. Journal of Chemical Physics, 1996, 105, 2710-2718.	1.2	50
7	On the Structuring of the Computational Chemistry Virtual Organization COMPCHEM. Lecture Notes in Computer Science, 2006, , 665-674.	1.0	50
8	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
9	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
10	Innovative computing and detailed properties of elementary reactions using time independent approaches. Computer Physics Communications, 1999, 116, 1-16.	3.0	36
11	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
12	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
13	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
14	An innovative synergistic grid approach to the computational study of protein aggregation mechanisms. Journal of Molecular Modeling, 2014, 20, 2226.	0.8	32
15	A potential energy surface for the Li+HCl reaction. Journal of Chemical Physics, 1988, 88, 181-190.	1.2	30
16	Potential energy representations in the bond order space. Chemical Physics, 1992, 168, 341-348.	0.9	30
17	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
18	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

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19	Wave packet calculations for the Cl + H2reaction. International Journal of Quantum Chemistry, 2004, 96, 562-567.	1.0	29
20	The last mile of molecular reaction dynamics virtual experiments: the case of the OH(N = 1â€“10) + CO(j =) Tj ETQq0 0 0 rgBT /Overlock	1.6	28
21	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
22	A LAGROBO strategy to fit potential energy surfaces: the OH+HCl reaction. Chemical Physics Letters, 2002, 360, 304-312.	1.2	27
23	An extension of the grid empowered molecular simulator to quantum reactive scattering. Journal of Computational Chemistry, 2012, 33, 708-714.	1.5	26
24	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
25	On the effect of increasing the total angular momentum on Li+HF reactivity. Chemical Physics Letters, 2000, 324, 466-474.	1.2	25
26	Thermal rate coefficients in collinear versus bent transition state reactions: the N+N₂case study. Physica Scripta, 2008, 78, 058116.	1.2	25
27	Methane production by CO2 hydrogenation reaction with and without solid phase catalysis. Fuel, 2017, 209, 802-811.	3.4	25
28	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
29	Vibrational deactivation mechanisms for O+2(v=1) colliding with Kr. Journal of Chemical Physics, 1988, 88, 4814-4818.	1.2	23
30	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
31	Quantum isotopic effects and reaction mechanisms: the Li+HF reaction. Physical Chemistry Chemical Physics, 2000, 2, 535-540.	1.3	22
32	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
33	Time-dependent wavepacket calculations for the system on a LEPS surface: inelastic and reactive probabilities. Molecular Physics, 2004, 102, 2237-2248.	0.8	22
34	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
35	A Nonorthogonal Coordinate Approach to Atom-Diatom Parallel Reactive Scattering Calculations. Collection of Czechoslovak Chemical Communications, 2003, 68, 307-330.	1.0	22
36	A detailed trajectory study of the OH+COâ†'H+CO2 reaction. Chemical Physics, 2007, 332, 162-175.	0.9	21

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37	Microscopic branching processes: The O + O₂ reaction and its relaxed potential representations. International Journal of Quantum Chemistry, 2010, 110, 358-367.	1.0	21
38	Calculated versus measured vibrational state specific reactivity of hydrogen atom + fluorine. The Journal of Physical Chemistry, 1993, 97, 8578-8582.	2.9	20
39	Full dimensional quantum versus semiclassical reactivity for the bent transition state reaction N+N2. Chemical Physics Letters, 2008, 464, 249-255.	1.2	20
40	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
41	The O + O2 reaction: quantum detailed probabilities and thermal rate coefficients. Theoretical Chemistry Accounts, 2009, 123, 249-256.	0.5	19
42	Parallel calculations of approximate 3D quantum cross sections: the Li + HF reaction. Chemical Physics Letters, 1991, 176, 280-286.	1.2	18
43	The potential energy surface of the Na(32S12)+HF(X1Î£+) reaction. Chemical Physics Letters, 1993, 202, 284-290.	1.2	18
44	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
45	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
46	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
47	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
48	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
49	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
50	MCTDH calculations on the rigid OH radical moving along a (10,0) carbon nanotube. Chemical Physics Letters, 2013, 575, 18-22.	1.2	16
51	Federation of Distributed and Collaborative Repositories and Its Application on Science Learning Objects. Lecture Notes in Computer Science, 2011, , 466-478.	1.0	16
52	On the all channels representation of the potential energy surface for reactive collisions. Chemical Physics Letters, 1989, 158, 87-94.	1.2	15
53	A Full Dimensional Quasiclassical Trajectory Study of Cl + CH4Rate Coefficientsâ€. Journal of Physical Chemistry A, 2004, 108, 8752-8758.	1.1	15
54	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

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55	Taxonomy Management in a Federation of Distributed Repositories: A Chemistry Use Case. Lecture Notes in Computer Science, 2012, , 358-370.	1.0	15
56	Two-configuration mc potential energy surface for the reaction of Mg with HF. Chemical Physics, 1986, 101, 55-65.	0.9	14
57	An approximate three-dimensional quantum-mechanical study of the Li+HFâ†'LiF+H reaction. Chemical Physics Letters, 1989, 158, 362-368.	1.2	14
58	Molecular-like behavior and vector correlations for the magnesium + hydrogen fluoride reaction. The Journal of Physical Chemistry, 1992, 96, 3587-3590.	2.9	14
59	Learning Objects Efficient Handling in a Federation of Science Distributed Repositories. Lecture Notes in Computer Science, 2014, , 615-626.	1.0	14
60	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
61	Two-configuration potential energy surface for the collinear Ca + HF â†' CaF + H reaction. Chemical Physics Letters, 1986, 126, 330-334.	1.2	13
62	An approximate estimate of the Li+HF reactivity. Chemical Physics Letters, 1987, 139, 140-144.	1.2	13
63	Li + HCl RIOSA cross section calculations on parallel computers. Theoretica Chimica Acta, 1991, 79, 191-198.	0.9	13
64	Rotational and alignment effects in a multisurface wavepacket calculation for the Cl + H2reaction. Physical Chemistry Chemical Physics, 2004, 6, 5000-5006.	1.3	13
65	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
66	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
67	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
68	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
69	The ECTN Virtual Education Community Prosumer Model for Promoting and Assessing Chemical Knowledge. Lecture Notes in Computer Science, 2018, , 533-548.	1.0	12
70	On the Franckâ€"Condon behavior of the H+Cl2reaction. Journal of Chemical Physics, 1987, 86, 5523-5533.	1.2	11
71	A Grid Molecular Simulator for E-Science. Lecture Notes in Computer Science, 2005, , 16-22.	1.0	11
72	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

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73	Non-Bornâ€“Oppenheimer MCTDH calculations on the confined H2+ molecular ion. Chemical Physics Letters, 2010, 500, 144-148.	1.2	11
74	Heavyâ€”heavyâ€”light limit and exchanged-atom isotopic effects in atomâ€”diatom reactivity. Chemical Physics Letters, 1992, 189, 138-143.	1.2	10
75	Where are embarrassingly parallel problems? The atom-diatom quasiclassical reactivity. Theoretica Chimica Acta, 1993, 84, 413-421.	0.9	10
76	Isotopic effects in the product vibrational distribution of the OH(OD)+HCl reaction. Chemical Physics Letters, 2003, 371, 223-228.	1.2	10
77	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
78	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
79	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
80	About the convergence of reactive infinite order sudden calculations on parallel computers. Journal of Chemical Physics, 1991, 95, 2218-2219.	1.2	9
81	Reaction and dissociation mechanism control: the H2â€‰+â€‰H2system. Physical Chemistry Chemical Physics, 2002, 4, 5007-5013.	1.3	9
82	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
83	Calculated versus measured product distributions of the OH+D 2 reaction. Molecular Physics, 2006, 104, 839-846.	0.8	9
84	A Multiscale Virtual Reality Approach to Chemical Experiments. Lecture Notes in Computer Science, 2003, , 324-330.	1.0	9
85	D+D 2 Quasiclassical rate constant calculations on parallel computers. Theoretica Chimica Acta, 1991, 79, 323-333.	0.9	8
86	Computational granularity and parallel models to scale up reactive scattering calculations. Computer Physics Communications, 2000, 128, 295-314.	3.0	8
87	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
88	A priori molecular virtual reality on EGEE grid. International Journal of Quantum Chemistry, 2010, 110, 446-453.	1.0	8
89	A quantum-classical study of the OH + H 2 reactive and inelastic collisions. Chemical Physics Letters, 2017, 674, 103-108.	1.2	8
90	Linear Algebra Computation Benchmarks on a Model Grid Platform. Lecture Notes in Computer Science, 2003, , 297-306.	1.0	8

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91	A multiproperty analysis of the OH+H2(D2,HD) potential energy surface. Chemical Physics, 2005, 308, 201-210.	0.9	7
92	A Molecular Dynamics Study of Ion Permeability Through Molecular Pores. Lecture Notes in Computer Science, 2005, , 1093-1100.	1.0	7
93	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
94	Quantum reactive scattering on innovative computing platforms. Computer Physics Communications, 2013, 184, 1372-1380.	3.0	7
95	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
96	Immersive Molecular Virtual Reality Based on X3D and Web Services. Lecture Notes in Computer Science, 2006, , 212-221.	1.0	7
97	A Web-Based Metacomputing Problem-Solving Environment for Complex Applications. Lecture Notes in Computer Science, 2000, , 111-122.	1.0	7
98	Macroscopic indicators for microscopic branching: The Be+HFâ†'BeF+H chemical reaction. Chemical Physics Letters, 1990, 168, 448-453.	1.2	6
99	Parallel calculations of quasiclassical rate constants: the H + H2 reaction. Chemical Physics Letters, 1991, 176, 273-279.	1.2	6
100	From parallel to distributed computing for reactive scattering calculations. International Journal of Quantum Chemistry, 1994, 52, 85-102.	1.0	6
101	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
102	Parallel quantum scattering calculations applied to the dynamics of elementary reactions. Lecture Notes in Computer Science, 1998, , 331-337.	1.0	6
103	Virtual Reality Applied to Molecular Sciences. Lecture Notes in Computer Science, 2004, , 827-836.	1.0	6
104	EoL: A Web-Based Distance Assessment System. Lecture Notes in Computer Science, 2004, , 854-862.	1.0	6
105	A Time Dependent Study of the Nitrogen Atom Nitrogen Molecule Reaction. Lecture Notes in Computer Science, 2004, , 357-365.	1.0	6
106	Quantum dynamics of H atom transmission across carbon nanotubes. Theoretical Chemistry Accounts, 2007, 118, 47-52.	0.5	6
107	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
108	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

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109	Fine Grain Parallelism for Discrete Variable Approaches to Wavepacket Calculations. Lecture Notes in Computer Science, 2002, , 918-925.	1.0	6
110	Efficient Workload Distribution Bridging HTC and HPC in Scientific Computing. Lecture Notes in Computer Science, 2012, , 345-357.	1.0	6
111	The impact of parallel computing on reactive scattering calculations. Computer Physics Communications, 1992, 70, 223-241.	3.0	5
112	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
113	Eigensolutions for one-dimensional cuts of bond order potentials. Chemical Physics Letters, 1997, 267, 403-410.	1.2	5
114	Rate coefficients under jet conditions. Plasma Sources Science and Technology, 1998, 7, 359-362.	1.3	5
115	Virtual Chemical Laboratories and Their Management on the Web. Lecture Notes in Computer Science, 2005, , 905-912.	1.0	5
116	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
117	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
118	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
119	Ion-Water Cluster Molecular Dynamics Using a Semiempirical Intermolecular Potential. Lecture Notes in Computer Science, 2015, , 355-370.	1.0	5
120	Kinetics Of The H + CH₂ â†' CH + H₂ Reaction At Low Temperature. Journal of Physical Chemistry A, 2019, 123, 7408-7419.	1.1	5
121	Towards a Grid Based Universal Molecular Simulator. , 2004, , 363-380.		5
122	Cloud and Local Servers for a Federation of Molecular Science Learning Object Repositories. Lecture Notes in Computer Science, 2019, , 359-373.	1.0	5
123	Mobile Device Access to Collaborative Distributed Repositories of Chemistry Learning Objects. Lecture Notes in Computer Science, 2016, , 443-454.	1.0	5
124	Investigation of Propane and Methane Bulk Properties Structure Using Two Different Force Fields. Lecture Notes in Computer Science, 2008, , 1052-1064.	1.0	5
125	Competing mechanisms and productsâ€™ properties for the Be+HF reaction. Journal of Chemical Physics, 1990, 93, 1082-1088.	1.2	4
126	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

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127	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
128	Integrating Learning and Assessment Using the Semantic Web. Lecture Notes in Computer Science, 2005, , 921-927.	1.0	4
129	Time Dependent Quantum Reactive Scattering on GPU. Lecture Notes in Computer Science, 2011, , 428-441.	1.0	4
130	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
131	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
132	Bond Order Potentials for a priori Simulations of Polyatomic Reactions. Lecture Notes in Computer Science, 2004, , 328-337.	1.0	3
133	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
134	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
135	An approximate quantum mechanical study of the N+Oâ†'NO++eâ^' associative ionisation. Chemical Physics Letters, 2013, 557, 43-48.	1.2	3
136	A Grid Implementation of Direct Semiclassical Calculations of Rate Coefficients. Lecture Notes in Computer Science, 2009, , 93-103.	1.0	3
137	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
138	Quantum Reactive Scattering Calculations on GPU. Lecture Notes in Computer Science, 2012, , 292-303.	1.0	3
139	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
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	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
142	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
143	Collisional O2 + N2 State-Selected Cross Sections for Open Science Cloud Reuse. Journal of Physical Chemistry A, 2020, 124, 6445-6457.	1.1	2
144	Atom-Bond Additive Potentials for Benzene-Rare Gas Clusters. Lecture Notes in Computer Science, 2006, , 721-730.	1.0	2

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145	Parallel skeletons and computational grain in quantum reactive scattering calculations. , 2002, , .		2
146	Sharing Learning Objects Between Learning Platforms and Repositories. Lecture Notes in Computer Science, 2018, , 804-816.	1.0	2
147	Distributed computing for quantum reactive scattering calculations. AIP Conference Proceedings, 1995, , .	0.3	1
148	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
149	EChemTest: The Assessment of Chemistry Knowledge. Nachrichten Aus Der Chemie, 2006, 54, 1272-1272.	0.0	1
150	An alternative distribution model for the Molecular Dynamics study of liquid Propane on a grid platform. , 2007, , .		1
151	Cooperative modelling and design on the computing grid: data, flux and knowledge interoperability. Journal of Molecular Modeling, 2013, 19, 4215-4222.	0.8	1
152	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
153	Methane Production from H2 + CO2 Reaction: An Open Molecular Science Case for Computational and Experimental Studies. Physchem, 2021, 1, 82-94.	0.5	1
154	Parallel Approaches to the Integration of the Differential Equations for Reactive Scattering. Lecture Notes in Computer Science, 2002, , 908-917.	1.0	1
155	Simulation of Methane Production from Carbon Dioxide on a Collaborative Research Infrastructure. Lecture Notes in Computer Science, 2016, , 319-333.	1.0	1
156	Fine Grain Parallelization of a Discrete Variable Wavepacket Calculation Using ASSIST-CL. Lecture Notes in Computer Science, 2004, , 437-444.	1.0	1
157	A Grid Implementation of Chimere: Ozone Production in Central Italy. Lecture Notes in Computer Science, 2009, , 115-129.	1.0	1
158	Time Independent 3D Quantum Reactive Scattering on MIMD Parallel Computers. Lecture Notes in Computer Science, 2000, , 338-345.	1.0	1
159	A Grid Implementation of Direct Quantum Calculations of Rate Coefficients. Lecture Notes in Computer Science, 2009, , 104-114.	1.0	1
160	A model for parallel one dimensional eigenvalues and eigenfunctions calculations. Lecture Notes in Computer Science, 1998, , 364-370.	1.0	1
161	Reactive Collisional Spectroscopy: Scalar and Vector Information From Numerically Intensive Computing. Laser Chemistry, 1991, 11, 169-175.	0.5	0
162	FITTING: A Portal to Fit Potential Energy Functionals to ab initio Points. Lecture Notes in Computer Science, 2007, , 358-365.	1.0	0

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163	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
164	The MPI Structure of Chimere. Lecture Notes in Computer Science, 2012, , 417-431.	1.0	0
165	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