RamÃ³n SayÃ³s

List of Publications by Year
in descending order

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100 papers	2,482 citations	172207 29 h-index	276539 41 g-index
100 all docs	100 docs citations	100 times ranked	1444 citing authors

#	Article	IF	Citations
1	Analysis of product Doppler-broadened profiles generated from photoinitiated bimolecular reactions. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 1427.	1.7	79
2	Ab initio ground potential energy surface, VTST and QCT study of the O(3P)+CH4(Xâ€‰1A1)â†'OH(Xâ€‰2Î)+CH3(Xâ€‰2A2â€³) reaction. Journal of Chemical Physics, 1999, 110, 7326-7338.	1.2	73
3	Atomic and molecular data for spacecraft re-entry plasmas. Plasma Sources Science and Technology, 2016, 25, 033004.	1.3	69
4	Critical effect of carbon vacancies on the reverse water gas shift reaction over vanadium carbide catalysts. Applied Catalysis B: Environmental, 2020, 267, 118719.	10.8	69
5	Theoretical investigation of the eight low-lying electronic states of thecis- andtrans-nitric oxide dimers and its isomerization using multiconfigurational second-order perturbation theory (CASPT2). Journal of Chemical Physics, 2000, 112, 6608-6624.	1.2	67
6	Dynamics of the N(4Su) + NO(Xâ€‰2Î) â†' N2(Xâ€‰1Î£g+) + O(3Pg) atmospheric reaction on the 3Aâ€˜ ground potential energy surface. I. Analytical potential energy surface and preliminary quasiclassical trajectory calculations. Journal of Chemical Physics, 1992, 97, 5542-5553.	1.2	60
7	Velocity-aligned photofragment dynamics: Stereodynamics in the reaction oxygen atom(1D) + nitrous oxide .fwdarw. nitric oxide + nitric oxide. The Journal of Physical Chemistry, 1991, 95, 8169-8174.	2.9	58
8	New analytical (2Aâ€²,4Aâ€²) surfaces and theoretical rate constants for the N(4S)+O2 reaction. Journal of Chemical Physics, 2002, 117, 670-679.	1.2	58
9	Quasiclassical trajectory study of the N(4Su) + O2 (X 3Î£â¯g)â†'NO (X 2Î) + O (3Pg) atmospheric reaction on the 2Aâ€² ground potential energy surface employing an analytical Sorbieâ€"Murrell potential. Chemical Physics, 1993, 172, 99-115.	0.9	54
10	Kinetic Monte Carlo simulations of the water gas shift reaction on Cu(1 1 1) from density functional theory based calculations. Journal of Catalysis, 2016, 333, 217-226.	3.1	53
11	Adsorption of Atomic Oxygen and Nitrogen at Î²-Cristobalite (100):Â A Density Functional Theory Study. Journal of Physical Chemistry B, 2005, 109, 14954-14964.	1.2	49
12	Ab initio derived analytical fits of the two lowest triplet potential energy surfaces and theoretical rate constants for the N(4S)+NO(Xâ€‰2Î) system. Journal of Chemical Physics, 2003, 119, 2545-2556.	1.2	48
13	Measurements of vector correlations in bimolecular reactions by laser-pump and probe techniques. Chemical Physics Letters, 1991, 182, 568-574.	1.2	44
14	A comparison between experimental, quantum and quasiclassical properties for the reaction. Chemical Physics, 1995, 191, 1-15.	0.9	43
15	Multiscale Study of the Mechanism of Catalytic CO₂ Hydrogenation: Role of the Ni(111) Facets. ACS Catalysis, 2020, 10, 8077-8089.	5.5	43
16	An analytical potential energy surface of the HClF (2Aâ€²) system based on ab initio calculations. Variational transition state theory study of the H+ClFâ†'F+HCl, Cl+HF and F+HClâ†'Cl+HF reactions and their deuterium isotope variants. Physical Chemistry Chemical Physics, 1999, 1, 947-956.	1.3	39
17	Quantum reactive scattering calculations of cross sections and rate constants for the N(2D)+O2(Xâ€‰3Î£gâ¯)â†'O(3P)+NO(Xâ€‰2Î) reaction. Journal of Chemical Physics, 2003, 118, 3111-3123.	1.2	38
18	Density Functional Theory-Based Adsorption Isotherms for Pure and Flue Gas Mixtures on Mg-MOF-74. Application in CO₂ Capture Swing Adsorption Processes. Journal of Physical Chemistry C, 2018, 122, 3945-3957.	1.5	38

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19	Assessing the usefulness of transition metal carbides for hydrogenation reactions. Chemical Communications, 2019, 55, 12797-12800.	2.2	37
20	Ab initio ground potential energy surface and quasiclassical trajectory study of the O(1D)+CH4(Xâ€Š1A1)â†'OH(Xâ€Š2Î)+CH3(Xâ€Š2A2â€³) reaction dynamics. Journal of Chemical Physics, 1999, 111, 8913-8924.	1.2	35
21	Quasiclassical dynamics and kinetics of the N+NOâ†'N2+O, NO+N atmospheric reactions. Journal of Chemical Physics, 2010, 132, 144304.	1.2	35
22	Optimal Faujasite structures for post combustion CO 2 capture and separation in different swing adsorption processes. Journal of CO2 Utilization, 2017, 19, 100-111.	3.3	35
23	Quantum real wave-packet dynamics of the N(S4)+NO(XÌƒÎ2)â†'N2(XÌƒÎ£g+1)+O(P3) reaction on the ground and first excited triplet potential energy surfaces: Rate constants, cross sections, and product distributions. Journal of Chemical Physics, 2006, 124, 174303.	1.2	34
24	DFT and kinetics study of O/O2 mixtures reacting over a graphite (0001) basal surface. Theoretical Chemistry Accounts, 2011, 128, 683-694.	0.5	34
25	Ab initio study of the two lowest triplet potential energy surfaces involved in the N(4S)+NO (Xâ€‰2Î) reaction. Journal of Chemical Physics, 2003, 118, 10602-10610.	1.2	33
26	Dynamics of the N(4Su)+NO(Xâ€‰2Î)â†'N2(Xâ€‰1Î£+g)+O(3Pg) atmospheric reaction on the3Aâ€˜ ground potential energy surface. II. The effect of reagent translational, vibrational, and rotational energies. Journal of Chemical Physics, 1993, 99, 1719-1733.	1.2	32
27	Quasiclassical trajectory study of the H+ClFâ†'F+HCl, Cl+HF and F+HClâ†'Cl+HF reactions and their deuterium isotope variants on a new (2Aâ€²) ab initio potential energy surface. Physical Chemistry Chemical Physics, 2000, 2, 523-533.	1.3	32
28	Potential Energy Surface of the O(1D) + N2O â†' 2NO, O2+ N2Reactions. Journal of Physical Chemistry A, 1997, 101, 1206-1215.	1.1	30
29	Influence of the Collision Energy on the O(1D) + RH â†' OH(X2Î) + R (RH = CH4, C2H6, C3H8) Reaction Dynamics:Â A Laser-Induced Fluorescence and Quasiclassical Trajectory Study. Journal of Physical Chemistry A, 2000, 104, 521-529.	1.1	30
30	Comparing the catalytic activity of the water gas shift reaction on Cu(3 2 1) and Cu(1 1 1) surfaces: Step sites do not always enhance the overall reactivity. Journal of Catalysis, 2016, 342, 75-83.	3.1	30
31	Kinetic Monte Carlo Simulations Unveil Synergic Effects at Work on Bifunctional Catalysts. ACS Catalysis, 2019, 9, 9117-9126.	5.5	30
32	Variational transition state calculation of the rate constants for the N(4Su)+O2(Xâ€ˆ3Î£gâ€˜)â†'NO(Xâ€ˆ2Î)+O(3Pg) reaction and its reverse between 300 and 5000 K. Chemical Physics Letters, 1998, 284, 101-108.	1.2	29
33	An analytical representation of the ground potential energy surface (2Aâ€²) of the H+Cl2â†'HCl+Cl and Cl+HClâ†'HCl+Cl reactions, based on ab initio calculations. Journal of Chemical Physics, 1998, 108, 3168-3177.	1.2	29
34	A theoretical approach to the O(1D)+H2O(Xâ€Šâ€Š1A1) reaction: Ab initio potential energy surface and quasiclassical trajectory dynamics study. Journal of Chemical Physics, 2000, 113, 6736-6747.	1.2	29
35	General concepts, assumptions, drawbacks, and misuses in kinetic <scp>M</scp>onte <scp>C</scp>arlo and microkinetic modeling simulations applied to computational heterogeneous catalysis. International Journal of Quantum Chemistry, 2018, 118, e25518.	1.0	28
36	Dynamics of the N(4S)+NO(Xâ€‰2Î)â†'N2(Xâ€‰1Î£+g)+O(3P) atmospheric reaction on the3Aâ€³ ground potential energy surface. III. Quantum dynamical study and comparison with quasiclassical and experimental results. Journal of Chemical Physics, 1995, 103, 4496-4508.	1.2	27

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37	Theoretical study of the dynamics, stereodynamics, and microscopic mechanism of the O(1D)+CH4(Xâ€‰1A1)â†'OH(Xâ€‰2Î)+CH3(Xâ€‰2A2â€³) reaction. Journal of Chemical Physics, 2000, 113, 6748-6759.	1.2	26
38	Quantum dynamics of the N(4S)+O2 reaction on the Xâ€‰2Aâ€² and aâ€‰4Aâ€² surfaces: Reaction probabilities, cross sections, rate constants, and product distributions. Journal of Chemical Physics, 2002, 117, 3647-3655.	1.2	26
39	Influence of collision energy on the dynamics of the reaction O(1D)â€‰+â€‰CH4(X1A1)â€‰â†'â€‰OH(X 2Î)â€‰+â€‰CH3(X 2A2 Physical Chemistry Chemical Physics, 2002, 4, 288-294.	1.3	25
40	On the use of quantum chemical methods as an additional tool in studying corrosion inhibitor substances. Corrosion Science, 1986, 26, 927-934.	3.0	24
41	Low energy dynamics, isotopic effects and detailed microscopic reaction mechanism of the ion-molecule reaction N+ (3P) + H2 â†' NH+ + H. Chemical Physics, 1989, 132, 137-151.	0.9	24
42	A quasiclassical trajectory study of the effect of the initial rovibrational level and relative translational energy of reactants on the dynamics of the N(4Su) + O2(X 3âˆ'â^'g) â†' NO(X 2Î) + O(3Pg) atmospheric reaction on the 2Aâ€² ground potential energy surface. Chemical Physics, 1993, 178, 287-303.	0.9	24
43	Orientational dependence of the N(4S)+ NO(X2Î) and N(4S)+ O2(X3Î£â€"g) reactions: comparison of the angle-dependent line-of-centres model with quasiclassical trajectories. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 3223-3234.	1.7	23
44	The lowest doublet and quartet potential energy surfaces involved in the N(4S)+O2 reaction. I. Ab initio study of the Cs-symmetry (2Aâ€²,â€Š4Aâ€²) abstraction and insertion mechanisms. Journal of Chemical Physics, 2001, 115, 1287-1297.	1.2	23
45	A comparison between experimental and theoretical excitation functions for the O++H2 (4Aâ€˜) system using trajectory calculations over a wide energy range. Journal of Chemical Physics, 1993, 98, 2927-2935.	1.2	22
46	Quantum mechanical and quasiclassical Bornâ€"Oppenheimer dynamics of the reaction N2 on the N2O and surfaces. Chemical Physics, 2012, 398, 81-89.	0.9	22
47	Unexpectedly large impact of van der Waals interactions on the description of heterogeneously catalyzed reactions: the water gas shift reaction on Cu(321) as a case example. Physical Chemistry Chemical Physics, 2016, 18, 2792-2801.	1.3	22
48	VTST kinetics study of the N(2D)+O2(X3Î£gâ^')â†'NO(X2Î)+O(3P,1D) reactions based on CASSCF and CASPT2 ab initio calculations including excited potential energy surfaces. Chemical Physics Letters, 2001, 335, 339-347.	1.2	21
49	Ab initio1Aâ€² ground potential energy surface and transition state theory kinetics study of the O(1D)+N2Oâ†'2NO, N2+O2(aâ€‰1Î”g) reactions. Journal of Chemical Physics, 2001, 115, 7015-7031.	1.2	21
50	Ab initiostudy of the O(1D)+CH4(Xâ€Š1A1)â†'OH(Xâ€Š2Î)+CH3(Xâ€Š2A2â€³) reaction: Ground and excited potential energy surfaces. Journal of Chemical Physics, 2003, 119, 9504-9512.	1.2	21
51	A density functional theory study of atomic oxygen and nitrogen adsorption over Î±-alumina (0001). Physical Chemistry Chemical Physics, 2007, 9, 5112.	1.3	21
52	Recombination and chemical energy accommodation coefficients from chemical dynamics simulations: O/O2 mixtures reacting over a Î²-cristobalite (001) surface. Physical Chemistry Chemical Physics, 2011, 13, 17494.	1.3	21
53	Calculated product state distributions for the H+HIâ†'H2+I reaction at 0.68 and 1.60 eV relative energies. Chemical Physics Letters, 1989, 164, 643-652.	1.2	20
54	Classical dynamics of the O(3P)+CS(X1Î£+)â†'CO(X1Î£+)+S(3P) reaction on the ground triplet potential energy surface. Chemical Physics, 1990, 141, 401-415.	0.9	20

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55	An ab initio analytical potential energy surface for the O(3P)+CS(Xâ€‰1Î£+)â†’CO(Xâ€‰1Î£+)+S(3P) reaction useful for kinetic and dynamical studies. Journal of Chemical Physics, 1996, 105, 10999-11006.	1.2	20
56	Quantum wave packet dynamics of the 1â€Š3Aâ€³â€‰N(4S)+NO(XÌƒâ€Š2Î)â†’N2(XÌƒâ€Š1Î£g+)+O(3P) reaction. Journal of Chemical Physics, 2003, 119, 7156-7162.	1.2	20
57	Eleyâ€“Rideal reaction dynamics between O atoms on Î²-cristobalite (100) surface: A new interpolated potential energy surface and classical trajectory study. Surface Science, 2009, 603, 2742-2751.	0.8	20
58	Ab initio, VTST, and QCT study of the 1â€Š2Aâ€³ potential energy surface of the N(2D)+O2(Xâ€Š3Î£gâ¯)â†’O(3P)+NO(Xâ€Š2Î) reaction. Journal of Chemical Physics, 2001, 115, 8838-8851.	1.2	19
59	The lowest doublet and quartet potential energy surfaces involved in the N(4S)+O2 reaction. II. Ab initio study of the C2v-symmetry insertion mechanism. Journal of Chemical Physics, 2002, 117, 680-692.	1.2	19
60	Classical dynamics study of atomic oxygen sticking on the Î²-cristobalite (1 0 0) surface. Surface Science, 2008, 602, 975-985.	0.8	19
61	A molecular dynamics simulation of hydrogen atoms collisions on an H-preadsorbed silica surface. Plasma Sources Science and Technology, 2014, 23, 045016.	1.3	19
62	Quasiclassical Trajectory Dynamics Study of Atomic Oxygen Collisions on an O-Preadsorbed Graphite (0001) Surface with a New Analytical Potential Energy Surface. Journal of Physical Chemistry C, 2012, 116, 13092-13103.	1.5	18
63	The dynamics of the O(1D)+N2Oâ†’NO+NO reaction revisited: a QCT study on model potential energy surfaces. Chemical Physics Letters, 1999, 300, 603-612.	1.2	17
64	Collision energy effects on the dynamics of the reaction O(3P)+CH4(X1A1)â†’OH(X2Î)+CH3(X2A2â€³). Chemical Physics Letters, 2001, 341, 608-618.	1.2	17
65	Ab initio CASPT2//CASSCF study of the O(1D)+H2O(Xâ€‰1A1) reaction. Journal of Chemical Physics, 2001, 115, 8828-8837.	1.2	17
66	Classical dynamics study of atomic oxygen over graphite (0001) with new interpolated and analytical potential energy surfaces. Computational and Theoretical Chemistry, 2012, 990, 132-143.	1.1	17
67	Ab initio, variational transition state theory and quasiclassical trajectory study on the lowest 2Aâ€² potential energy surface involved in the N(2D)+O2(Xâ€Š3Î£gâ¯)â†’O(3P)+NO(Xâ€Š2Î) atmospheric reaction. Journal of Chemical Physics, 2001, 115, 2530-2539.	1.2	16
68	Computational simulation study of the influence of faujasite Si/Al ratio on CO2 capture by temperature swing adsorption. Journal of CO2 Utilization, 2017, 21, 261-269.	3.3	16
69	B(2P)+ H2O (X1A1): a quasi-classical 3D trajectory calculation. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 1057-1068.	1.7	15
70	Effect of reagent rotation on the dynamics of the O+ + H2 ionâ€“molecule reaction and isotopic variants. Chemical Physics Letters, 1993, 204, 578-586.	1.2	15
71	Assessing the Activity of Ni Clusters Supported on TiC(001) toward CO₂ and H₂ Dissociation. Journal of Physical Chemistry C, 2021, 125, 12019-12027.	1.5	15
72	Dynamics of the Oxygen Molecules Scattered from the Graphite (0001) Surface and Comparison with Experimental Data. Journal of Physical Chemistry C, 2012, 116, 21482-21488.	1.5	14

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73	Classical dynamics study of the H+BrCh3 â†’ HBr+CH3 reaction. Chemical Physics, 1985, 98, 409-419.	0.9	13
74	Ab initio ground potential energy surface (3Aâ€³) for the O(3P)+N2O reaction and kinetics study. Journal of Chemical Physics, 2001, 115, 2540-2549.	1.2	13
75	Crossed molecular beams study of the M+(1S)+Na(3 2S)â†’M+(1S)+Na(3 2P) collision systems (M+=Li+, Na+,) Tj ETQq1 1 0.784314 rgBT	1.2	12
76	Ab initio and DFT study of the ground potential energy surface for the ()+â†’2 reaction. Chemical Physics Letters, 2001, 343, 119-129.	1.2	12
77	Ab initio and kinetics study of the ground 1Aâ€³ potential energy surface of the O(1D)+N2Oâ†’2NO, N2+O2(a1Î”g) reactions. Chemical Physics Letters, 2002, 355, 123-132.	1.2	12
78	Ab initio study of the lowest 3Aâ€² and 3Aâ€³ potential energy surfaces involved in the O(3P) + CS(X1Î£+) â†’ CO(X) Tj ETQq0 0 0 rgBT	1.2	11
79	A QCT study of the microscopic mechanisms proceeding via the ground PES of the O(1D)+H2 (X1Î£g+)â†’OH(X2Î)+H(2S) reaction. Chemical Physics Letters, 2003, 380, 123-134.	1.2	11
80	Influence of collision energy on the N(2D)+O2â†’O(3P)+NO reaction dynamics: A quasiclassical trajectory study involving four potential energy surfaces. Journal of Chemical Physics, 2003, 119, 10040-10047.	1.2	11
81	Zeolite-encapsulated single-atom catalysts for efficient CO2 conversion. Journal of CO2 Utilization, 2021, 54, 101777.	3.3	11
82	Influence of the potential energy surface on the reaction cross section: the K + HF â†’ KF + H system. Chemical Physics, 1995, 200, 289-308.	0.9	8
83	Structural, electronic, and magnetic properties of Ni nanoparticles supported on the TiC(001) surface. Physical Chemistry Chemical Physics, 2020, 22, 26145-26154.	1.3	8
84	Theoretical study of the reaction H + ClCH3 â†’ HCl + CH3. Chemical Physics, 1985, 93, 265-275.	0.9	7
85	A theoretical study of the addition of atomic boron to water.. Computational and Theoretical Chemistry, 1988, 166, 301-306.	1.5	7
86	Quasi-classical trajectory study of the dynamics of the reaction O(3P)+CS2(X1âˆ+g)â†’CS(X1âˆ+)+SO(X3âˆâˆ) using two model potential energy surfaces. Chemical Physics, 1992, 161, 99-126.	0.9	7
87	Dynamics of the Four-Atom BO + H2 â†’ HBO + H Reaction:â€‰ Potential Energy Surface and Reaction Selectivity from QCT Calculations. Journal of Physical Chemistry A, 1997, 101, 8877-8886.	1.1	7
88	Quasiclassical Trajectory Study of Molecular Alignment Effects on the Dynamics of the Reactions of Cl, Br, and I with H2. Journal of Physical Chemistry A, 1997, 101, 7513-7521.	1.1	7
89	Theoretical Study of the Dynamics and Kinetics of the O + CS â†’ CO + S Chemical Laser Reaction, Where CO Shows a Very High Vibrational Excitation. Journal of Physical Chemistry A, 2012, 116, 11783-11795.	1.1	7
90	Transition metal atoms encapsulated within microporous Silicalite-1 zeolite: A systematic computational study. Microporous and Mesoporous Materials, 2020, 308, 110462.	2.2	7

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91	On the reaction Si+(2P) + H2(X1Î£+g) â†' SiH+ + H. I. Ab initio potential energy surfaces. Chemical Physics, 1987, 113, 417-424.	0.9	6
92	Stereodynamical Studies of Velocity Aligned Photofragments. Laser Chemistry, 1991, 11, 265-272.	0.5	6
93	Ab initio, VTST and QCT study of the potential energy surface implied in the reaction. Chemical Physics Letters, 2002, 360, 521-533.	1.2	6
94	Elementary Reaction Processes Involving Atomic and Molecular Oxygen on ZrB2(0001) Surface. Journal of Physical Chemistry C, 2013, 117, 5831-5839.	1.5	5
95	ReaxFF molecular dynamics simulations of CO collisions on an O-preadsorbed silica surface. Journal of Molecular Modeling, 2014, 20, 2160.	0.8	5
96	Influence of Collision Energy on the Nascent OH(X2Î,vâ€˜Ââ€˜ = 0â^'4) Product Energetics for the Reaction of O(1D) with Ethane. A Laser-Induced Fluorescence and Quasiclassical Trajectory Study. Journal of Physical Chemistry A, 2001, 105, 9834-9844.	1.1	4
97	A MNDO approach to the elementary reactions of atomic hydrogen with monosubstituted halomethanes (CH3X, X î—» Cl, Br, I). Chemical Physics, 1986, 104, 49-56.	0.9	3
98	Nascent OH (X2Î) product state distributions from the reaction of O(1 D) with ethylene.. Chemical Physics Letters, 2001, 346, 69-80.	1.2	3
99	Molecular dynamics study of hydrogen atom recombination over silica, based on a new analytical DFT potential energy surface. , 2012, , .		3
100	Theoretical Characterization of Transition State Dynamical Resonances in Heavyâ€“Lightâ€“Heavy Reactions. Laser Chemistry, 1991, 11, 291-302.	0.5	0