Bastiaan J. Braams

List of Publications by Year
in descending order

108	6,614	61984	62596
papers	citations	43 h-index	80 g-index

121	121	121	3910
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	EUROfusion-theory and advanced simulation coordination (E-TASC): programme and the role of high performance computing. Plasma Physics and Controlled Fusion, 2022, 64, 034005.	2.1	2
2	Data on erosion and hydrogen fuel retention in Beryllium plasma-facing materials. Nuclear Materials and Energy, 2021, 27, 100994.	1.3	21
3	Neutral dissociation of methane by electron impact and a complete and consistent cross section set. Plasma Sources Science and Technology, 2021, 30, 075012.	3.1	10
4	Iso-nuclear tungsten dielectronic recombination rates for use in magnetically-confined fusion plasmas. Atomic Data and Nuclear Data Tables, 2018, 119, 250-262.	2.4	11
5	QDB: a new database of plasma chemistries and reactions. Plasma Sources Science and Technology, 2017, 26, 055014.	3.1	42
6	Equilibrium clumped-isotope effects in doubly substituted isotopologues of ethane. Geochimica Et Cosmochimica Acta, 2017, 197, 14-26.	3.9	15
7	The virtual atomic and molecular data centre (VAMDC) consortium. Journal of Physics B: Atomic, Molecular and Optical Physics, 2016, 49, 074003.	1.5	120
8	Uncertainty estimates for theoretical atomic and molecular data. Journal Physics D: Applied Physics, 2016, 49, 363002.	2.8	66
9	Light element atom, molecule and radical behaviour in the divertor and edge plasma regions. Journal of Physics: Conference Series, 2015, 576, 011001.	0.4	5
10	Uncertainty Quantification of theoretical atomic and molecular collisional data. Journal of Physics: Conference Series, 2015, 635, 052020.	0.4	1
11	Analytical potential energy surface for O+C2H2 system. Chemical Physics Letters, 2013, 588, 22-26.	2.6	4
12	Coordinated activities on evaluation of collisional data for fusion applications. , 2013, , .		0
13	Databases and coordinated research projects at the IAEA on atomic processes in plasmas. , 2012, , .		0
14	The Dynamics of Allyl Radical Dissociation. Journal of Physical Chemistry A, 2011, 115, 6797-6804.	2.5	19
15	Comparative study of the dust particle population sampled during four consecutive campaigns in full-tungsten ASDEX Upgrade. Physica Scripta, 2011, T145, 014021.	2.5	19
16	Flexible, ab initio potential, and dipole moment surfaces for water. I. Tests and applications for clusters up to the 22-mer. Journal of Chemical Physics, 2011, 134, 094509.	3.0	238
17	Coordinated Research Projects of the IAEA Atomic and Molecular Data Unit. , 2011, , .		3
18	Depression of reactivity by the collision energy in the single barrier HÂ+ÂCD ₄ Âà†'ÂHDÂ+ÂCD ₃ reaction. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 12782-12785.	7.1	105

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19	Global potential energy surfaces for O(P3)+H2O(A11) collisions. Journal of Chemical Physics, 2010, 133, 164312.	3.0	23
20	Evidence for Vinylidene Production in the Photodissociation of the Allyl Radical. Journal of Physical Chemistry Letters, 2010, 1, 1875-1880.	4.6	40
21	Shared-Proton Mode Lights up the Infrared Spectrum of Fluxional Cations H₅⁺ and D₅⁺. Journal of Physical Chemistry Letters, 2010, 1, 758-762.	4.6	52
22	Ab-Initio-Based Potential Energy Surfaces for Complex Molecules and Molecular Complexes. Journal of Physical Chemistry Letters, 2010, 1, 1866-1874.	4.6	97
23	Ro-vibrational spectra of C₂H₂based on variational nuclear motion calculations. Molecular Physics, 2010, 108, 1973-1990.	1.7	20
24	Full-dimensional ab initio potential energy surface and vibrational configuration interaction calculations for vinyl. Journal of Chemical Physics, 2009, 130, 174301.	3.0	54
25	Photochemical reactions of the low-lying excited states of formaldehyde: T1/S intersystem crossings, characteristics of the S1 and T1 potential energy surfaces, and a global T1 potential energy surface. Journal of Chemical Physics, 2009, 130, 114304.	3.0	37
26	Proton affinity and enthalpy of formation of formaldehyde. International Journal of Quantum Chemistry, 2009, 109, 2393-2409.	2.0	33
27	Ab Initio Calculation of the Photoelectron Spectra of the Hydroxycarbene Diradicals. Journal of Physical Chemistry A, 2009, 113, 7802-7809.	2.5	28
28	Full-dimensional, ab initio potential energy and dipole moment surfaces for water. Journal of Chemical Physics, 2009, 131, 054511.	3.0	133
29	Permutationally invariant potential energy surfaces in high dimensionality. International Reviews in Physical Chemistry, 2009, 28, 577-606.	2.3	730
30	Quasiclassical trajectory calculations of the HO2 + NO reaction on a global potential energy surface. Physical Chemistry Chemical Physics, 2009, 11, 4722.	2.8	25
31	Accurate ab initio and â€œhybridâ€•potential energy surfaces, intramolecular vibrational energies, and classical ir spectrum of the water dimer. Journal of Chemical Physics, 2009, 130, 144314.	3.0	162
32	Accurate ab initio potential energy surface, dynamics, and thermochemistry of the F+CH4â†'HF+CH3 reaction. Journal of Chemical Physics, 2009, 130, 084301.	3.0	130
33	AbÂinitio modeling of molecular IR spectra of astrophysical interest: application to CH₄. Astronomy and Astrophysics, 2009, 495, 655-661.	5.1	46
34	Potential energy surface and quantum dynamics study of rovibrational states for HO3 (Xâ€‰2Aâ€³). Physical Chemistry Chemical Physics, 2008, 10, 3150.	2.8	31
35	Variational calculation of second-order reduced density matrices by strong N-representability conditions and an accurate semidefinite programming solver. Journal of Chemical Physics, 2008, 128, 164113.	3.0	62
36	â€œRoamingâ€•Dynamics in CH₃CHO Photodissociation Revealed on a Global Potential Energy Surface. Journal of Physical Chemistry A, 2008, 112, 9344-9351.	2.5	84

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37	Accurate ab Initio Structure, Dissociation Energy, and Vibrational Spectroscopy of the Fâ^'â^'CH4 Anion Complex. Journal of Physical Chemistry A, 2008, 112, 7466-7472.	2.5	25
38	Probing the Structure of CH₅⁺ by Dissociative Charge Exchange. Journal of the American Chemical Society, 2008, 130, 3730-3731.	13.7	22
39	Full-dimensional quantum calculations of ground-state tunneling splitting of malonaldehyde using an accurate ab initio potential energy surface. Journal of Chemical Physics, 2008, 128, 224314.	3.0	149
40	Roaming is the dominant mechanism for molecular products in acetaldehyde photodissociation. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 12719-12724.	7.1	183
41	New ab initio potential energy surface and the vibration-rotation-tunneling levels of (H2O)2 and (D2O)2. Journal of Chemical Physics, 2008, 128, 034312.	3.0	104
42	Vibrational ground state properties of H5+ and its isotopomers from diffusion Monte Carlo calculations. Journal of Chemical Physics, 2008, 128, 104318.	3.0	48
43	<scp>MULTIMODE</scp> quantum calculations of intramolecular vibrational energies of the water dimer and trimer using ab initio-based potential energy surfaces. Journal of Chemical Physics, 2008, 128, 071101.	3.0	59
44	The theoretical prediction of infrared spectra of trans- and cis-hydroxycarbene calculated using full dimensional ab initio potential energy and dipole moment surfaces. Journal of Chemical Physics, 2008, 128, 204310.	3.0	33
45	Quasiclassical trajectory calculations of the OH+NO2 association reaction on a global potential energy surface. Journal of Chemical Physics, 2007, 127, 104310.	3.0	19
46	Quantum mechanical correlation functions, maximum entropy analytic continuation, and ring polymer molecular dynamics. Journal of Chemical Physics, 2007, 127, 174108.	3.0	64
47	Ab Intio Based Potential Energy Surfaces and Franckâ^'Condon Analysis of Ionization Thresholds of Cyclic-C3H and Linear-C3Hâ€. Journal of Physical Chemistry A, 2007, 111, 4056-4061.	2.5	7
48	Quasiclassical Trajectory Calculations of Acetaldehyde Dissociation on a Global Potential Energy Surface Indicate Significant Non-transition State Dynamics. Journal of Physical Chemistry A, 2007, 111, 8282-8285.	2.5	89
49	Quasiclassical Trajectory Study of the CH3++ HD â†' CH2D++ H2Reactionâ€. Journal of Physical Chemistry A, 2007, 111, 6658-6664.	2.5	11
50	The T 1 and T 2 Representability Conditions. Advances in Chemical Physics, 2007, , 93-101.	0.3	15
51	A Combined Experimental and Computational Study on the Ionization Energies of the Cyclic and Linear C3H Isomers. ChemPhysChem, 2007, 8, 1236-1239.	2.1	32
52	Large-scale semidefinite programs in electronic structure calculation. Mathematical Programming, 2007, 109, 553-580.	2.4	55
53	Potential energy surface and MULTIMODE vibrational analysis of C2H3+. Journal of Chemical Physics, 2006, 125, 224306.	3.0	35
54	Ab Initio Potential Energy and Dipole Moment Surfaces of (H2O)2â€. Journal of Physical Chemistry A, 2006, 110, 445-451.	2.5	115

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55	An ab Initio Based Global Potential Energy Surface Describing CH5+â†' CH3++ H2â€. Journal of Physical Chemistry A, 2006, 110, 1569-1574.	2.5	97
56	Simple Hamiltonians which exhibit drastic failures by variational determination of the two-particle reduced density matrix with some well known N-representability conditions. Journal of Chemical Physics, 2006, 125, 244109.	3.0	8
57	Sum rule constraints on Kubo-transformed correlation functions. Chemical Physics Letters, 2006, 418, 179-184.	2.6	21
58	Plasma Edge Physics with B2-Eirene. Contributions To Plasma Physics, 2006, 46, 3-191.	1.1	455
59	Quasiclassical trajectory calculations of the reaction C+C2H2â†'l-C3H, c-C3H+H, C3+H2 using full-dimensional triplet and singlet potential energy surfaces. Journal of Chemical Physics, 2006, 125, 081101.	3.0	32
60	On the short-time limit of ring polymer molecular dynamics. Journal of Chemical Physics, 2006, 125, 124105.	3.0	131
61	An ab initio potential surface describing abstraction and exchange for H+CH4. Journal of Chemical Physics, 2006, 124, 021104.	3.0	79
62	Ab initio global potential-energy surface for H5+â†'H3++H2. Journal of Chemical Physics, 2005, 122, 224307.	3.0	106
63	CONSTRUCTION OF A GLOBAL POTENTIAL ENERGY SURFACE FROM NOVEL AB INITIO MOLECULAR DYNAMICS FOR THE O(3P) + C3H3 REACTION. Journal of Theoretical and Computational Chemistry, 2005, 04, 163-173.	1.8	12
64	Ab initio potential energy and dipole moment surfaces for H5O2+. Journal of Chemical Physics, 2005, 122, 044308.	3.0	257
65	Quantum and classical studies of vibrational motion of CH5+ on a global potential energy surface obtained from a novel ab initio direct dynamics approach. Journal of Chemical Physics, 2004, 121, 4105-4116.	3.0	95
66	The reduced density matrix method for electronic structure calculations and the role of three-index representability conditions. Journal of Chemical Physics, 2004, 120, 2095-2104.	3.0	220
67	Simulation of the Edge Plasma in Tokamaks. Physica Scripta, 2004, , 7.	2.5	42
68	The National Transport Code Collaboration Module Library. Computer Physics Communications, 2004, 164, 108-113.	7.5	20
69	Quantum Calculations of Vibrational Energies of H3O2-on an ab Initio Potential. Journal of the American Chemical Society, 2004, 126, 5042-5043.	13.7	77
70	Ab Initio Diffusion Monte Carlo Calculations of the Quantum Behavior of CH5+ in Full Dimensionality. Journal of Physical Chemistry A, 2004, 108, 4991-4994.	2.5	87
71	Diffusion of excitons in systems with non-planar geometry: theory. Chemical Physics, 2003, 288, 105-112.	1.9	5
72	Classical and quasiclassical spectral analysis of CH5+ using an ab initio potential energy surface. Journal of Chemical Physics, 2003, 119, 8790-8793.	3.0	97

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73	Steady state advanced scenarios at ASDEX Upgrade. Plasma Physics and Controlled Fusion, 2002, 44, B69-B83.	2.1	108
74	On using low-order Hermite interpolation in `direct dynamics' calculations of vibrational energies using the code `MULTIMODE'. Chemical Physics Letters, 2001, 342, 636-642.	2.6	31
75	A local interpolation method for direct classical dynamics calculations. Journal of Chemical Physics, 2001, 115, 11021-11024.	3.0	10
76	The KSTAR project: An advanced steady state superconducting tokamak experiment. Nuclear Fusion, 2000, 40, 575-582.	3.5	168
77	B2-solps5.0: SOL transport code with drifts and currents. Contributions To Plasma Physics, 2000, 40, 328-333.	1.1	3
78	Scrape off layer modelling studies for SST-I. Journal of Nuclear Materials, 1999, 266-269, 726-731.	2.7	3
79	Modeling of neutral plasma in a divertor in the fluid-kinetic transition. Contributions To Plasma Physics, 1998, 38, 319-324.	1.1	14
80	Divertor tokamak operation at high densities on ASDEX Upgrade. Plasma Physics and Controlled Fusion, 1997, 39, B19-B38.	2.1	17
81	Progress in Integrated 2â€Ð Models for Analysis of Scrapeâ€Off Layer Transport Physics. Contributions To Plasma Physics, 1996, 36, 105-116.	1.1	31
82	Theory and Modelling of Time Dependent Phenomena in the Plasma Edge. Contributions To Plasma Physics, 1996, 36, 150-160.	1.1	16
83	Implementation into B2 of a 21-moment description for the parallel transport. Contributions To Plasma Physics, 1996, 36, 192-196.	1.1	20
84	Power Balance in the ITER Plasma and Divertor. Contributions To Plasma Physics, 1996, 36, 240-244.	1.1	9
85	Radiative Divertor Modelling for ITER and TPX. Contributions To Plasma Physics, 1996, 36, 276-281.	1.1	104
86	Numerical Simulation of the ITER Gaseous Divertor with the B2.5 Code. Contributions To Plasma Physics, 1996, 36, 282-287.	1.1	1
87	2D modelling of the ASDEX-Upgrade scrape-off layer and divertor plasma. Journal of Nuclear Materials, 1995, 220-222, 558-562.	2.7	34
88	Divertor design for the tokamak physics experiment. Journal of Nuclear Materials, 1995, 220-222, 698-702.	2.7	7
89	Analysis of cold divertor concepts for ITER. Journal of Nuclear Materials, 1995, 220-222, 1076-1080.	2.7	29
90	Up-down symmetry in double null divertor experiments and magnetic field topology. Nuclear Fusion, 1995, 35, 297-304.	3.5	11

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91	Assessment of critical physical assumptions in consistent 2D plasma edge modelling. Journal of Nuclear Materials, 1992, 196-198, 466-471.	2.7	11
92	B2-EIRENE simulation of ASDEX and ASDEX-Upgrade scrape-off layer plasmas. Journal of Nuclear Materials, 1992, 196-198, 810-815.	2.7	145
93	Scrape-off layer modeling using coupled plasma and neutral transport codes. Journal of Nuclear Materials, 1992, 196-198, 894-898.	2.7	6
94	Extensions of B2 for the Simulation of ASDEX â€" Upgrade Scrapeâ€off Layer Plasmas. Contributions To Plasma Physics, 1992, 32, 450-455.	1.1	18
95	Parameter Dependence of the Edge and Divertor Plasma in Asdexâ€Upgrade. Contributions To Plasma Physics, 1992, 32, 456-461.	1.1	2
96	The interpretation of tokamak magnetic diagnostics. Plasma Physics and Controlled Fusion, 1991, 33, 715-748.	2.1	95
97	TOkamak Edge Studies with A 2D Multifluid Code. Contributions To Plasma Physics, 1990, 30, 95-100.	1.1	10
98	Two-dimensional fluid simulations of the ITER SOL plasma. Journal of Nuclear Materials, 1990, 176-177, 909-915.	2.7	20
99	Compact ignition tokamak edge and divertor modeling. , 1990, , .		1
100	Conductivity of a relativistic plasma. Physics of Fluids B, 1989, 1, 1355-1368.	1.7	75
101	Tokamak edge modeling and comparison with experiment in ASDEX. Plasma Physics and Controlled Fusion, 1989, 31, 1551-1568.	2.1	75
102	2 D Tokamak Edge Simulation Including Impurities. Contributions To Plasma Physics, 1988, 28, 373-378.	1.1	5
103	Differential form of the collision integral for a relativistic plasma. Physical Review Letters, 1987, 59, 1817-1820.	7.8	43
104	Fast determination of plasma parameters through function parametrization. Nuclear Fusion, 1986, 26, 699-708.	3.5	66
105	Magnetohydrodynamic equilibrium calculations using multigrid. Lecture Notes in Mathematics, 1986, , 38-51.	0.2	0
106	Modelling of the boundary plasma of large tokamaks. Journal of Nuclear Materials, 1984, 121, 75-81.	2.7	35
107	Nonadiabatic particle response in toroidal geometry. Physics of Fluids, 1982, 25, 1871.	1.4	8
108	Edge plasma analyses for KSTAR divertor design. , 0, , .		1