

# Bastiaan J. Braams

## List of Publications by Year in descending order

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108  
papers

6,614  
citations

61984

43  
h-index

62596

80  
g-index

121  
all docs

121  
docs citations

121  
times ranked

3910  
citing authors

#	ARTICLE	IF	CITATIONS
1	Permutationally invariant potential energy surfaces in high dimensionality. <i>International Reviews in Physical Chemistry</i> , 2009, 28, 577-606.	2.3	730
2	Plasma Edge Physics with B2-Eirene. <i>Contributions To Plasma Physics</i> , 2006, 46, 3-191.	1.1	455
3	Ab initio potential energy and dipole moment surfaces for H5O2+. <i>Journal of Chemical Physics</i> , 2005, 122, 044308.	3.0	257
4	Flexible, <i>ab initio</i> potential, and dipole moment surfaces for water. I. Tests and applications for clusters up to the 22-mer. <i>Journal of Chemical Physics</i> , 2011, 134, 094509.	3.0	238
5	The reduced density matrix method for electronic structure calculations and the role of three-index representability conditions. <i>Journal of Chemical Physics</i> , 2004, 120, 2095-2104.	3.0	220
6	Roaming is the dominant mechanism for molecular products in acetaldehyde photodissociation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 12719-12724.	7.1	183
7	The KSTAR project: An advanced steady state superconducting tokamak experiment. <i>Nuclear Fusion</i> , 2000, 40, 575-582.	3.5	168
8	Accurate <i>ab initio</i> and $\hat{c}$ -hybrid potential energy surfaces, intramolecular vibrational energies, and classical ir spectrum of the water dimer. <i>Journal of Chemical Physics</i> , 2009, 130, 144314.	3.0	162
9	Full-dimensional quantum calculations of ground-state tunneling splitting of malonaldehyde using an accurate <i>ab initio</i> potential energy surface. <i>Journal of Chemical Physics</i> , 2008, 128, 224314.	3.0	149
10	B2-EIRENE simulation of ASDEX and ASDEX-Upgrade scrape-off layer plasmas. <i>Journal of Nuclear Materials</i> , 1992, 196-198, 810-815.	2.7	145
11	Full-dimensional, <i>ab initio</i> potential energy and dipole moment surfaces for water. <i>Journal of Chemical Physics</i> , 2009, 131, 054511.	3.0	133
12	On the short-time limit of ring polymer molecular dynamics. <i>Journal of Chemical Physics</i> , 2006, 125, 124105.	3.0	131
13	Accurate <i>ab initio</i> potential energy surface, dynamics, and thermochemistry of the $F+CH_4 \rightarrow HF+CH_3$ reaction. <i>Journal of Chemical Physics</i> , 2009, 130, 084301.	3.0	130
14	The virtual atomic and molecular data centre (VAMDC) consortium. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2016, 49, 074003.	1.5	120
15	Ab Initio Potential Energy and Dipole Moment Surfaces of (H2O) <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 2006, 110, 445-451.	2.5	115
16	Steady state advanced scenarios at ASDEX Upgrade. <i>Plasma Physics and Controlled Fusion</i> , 2002, 44, B69-B83.	2.1	108
17	Ab initio global potential-energy surface for H5 <sup>+</sup> H3 <sup>++</sup> H2. <i>Journal of Chemical Physics</i> , 2005, 122, 224307.	3.0	106
18	Depression of reactivity by the collision energy in the single barrier H <sub>4</sub> <sup>+</sup> H <sub>3</sub> <sup>++</sup> H <sub>2</sub> reaction. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 12782-12785.	7.1	105

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19	Radiative Divertor Modelling for ITER and TPX. Contributions To Plasma Physics, 1996, 36, 276-281.	1.1	104
20	New <i>ab initio</i> potential energy surface and the vibration-rotation-tunneling levels of (H <sub>2</sub> O) <sub>2</sub> and (D <sub>2</sub> O) <sub>2</sub> . Journal of Chemical Physics, 2008, 128, 034312.	3.0	104
21	Classical and quasiclassical spectral analysis of CH <sub>5</sub> <sup>+</sup> using an <i>ab initio</i> potential energy surface. Journal of Chemical Physics, 2003, 119, 8790-8793.	3.0	97
22	An <i>ab Initio</i> Based Global Potential Energy Surface Describing CH <sub>5</sub> <sup>+</sup> CH <sub>3</sub> <sup>++</sup> H <sub>2</sub> . Journal of Physical Chemistry A, 2006, 110, 1569-1574.	2.5	97
23	<i>Ab-Initio</i> -Based Potential Energy Surfaces for Complex Molecules and Molecular Complexes. Journal of Physical Chemistry Letters, 2010, 1, 1866-1874.	4.6	97
24	The interpretation of tokamak magnetic diagnostics. Plasma Physics and Controlled Fusion, 1991, 33, 715-748.	2.1	95
25	Quantum and classical studies of vibrational motion of CH <sub>5</sub> <sup>+</sup> on a global potential energy surface obtained from a novel <i>ab initio</i> direct dynamics approach. Journal of Chemical Physics, 2004, 121, 4105-4116.	3.0	95
26	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
27	<i>Ab Initio</i> Diffusion Monte Carlo Calculations of the Quantum Behavior of CH <sub>5</sub> <sup>+</sup> in Full Dimensionality. Journal of Physical Chemistry A, 2004, 108, 4991-4994.	2.5	87
28	“Roaming” Dynamics in CH <sub>3</sub> CHO Photodissociation Revealed on a Global Potential Energy Surface. Journal of Physical Chemistry A, 2008, 112, 9344-9351.	2.5	84
29	An <i>ab initio</i> potential surface describing abstraction and exchange for H+CH <sub>4</sub> . Journal of Chemical Physics, 2006, 124, 021104.	3.0	79
30	Quantum Calculations of Vibrational Energies of H <sub>3</sub> O <sub>2</sub> -on an <i>ab Initio</i> Potential. Journal of the American Chemical Society, 2004, 126, 5042-5043.	13.7	77
31	Conductivity of a relativistic plasma. Physics of Fluids B, 1989, 1, 1355-1368.	1.7	75
32	Tokamak edge modeling and comparison with experiment in ASDEX. Plasma Physics and Controlled Fusion, 1989, 31, 1551-1568.	2.1	75
33	Fast determination of plasma parameters through function parametrization. Nuclear Fusion, 1986, 26, 699-708.	3.5	66
34	Uncertainty estimates for theoretical atomic and molecular data. Journal Physics D: Applied Physics, 2016, 49, 363002.	2.8	66
35	Quantum mechanical correlation functions, maximum entropy analytic continuation, and ring polymer molecular dynamics. Journal of Chemical Physics, 2007, 127, 174108.	3.0	64
36	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

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37	<sc>MULTIMODE</sc> quantum calculations of intramolecular vibrational energies of the water dimer and trimer using <i>ab initio</i>-based potential energy surfaces. Journal of Chemical Physics, 2008, 128, 071101.	3.0	59
38	Large-scale semidefinite programs in electronic structure calculation. Mathematical Programming, 2007, 109, 553-580.	2.4	55
39	Full-dimensional <i>ab initio</i> potential energy surface and vibrational configuration interaction calculations for vinyl. Journal of Chemical Physics, 2009, 130, 174301.	3.0	54
40	Shared-Proton Mode Lights up the Infrared Spectrum of Fluxional Cations H<sub>5</sub><sup>+</sup> and D<sub>5</sub><sup>+</sup>. Journal of Physical Chemistry Letters, 2010, 1, 758-762.	4.6	52
41	Vibrational ground state properties of H5+ and its isotopomers from diffusion Monte Carlo calculations. Journal of Chemical Physics, 2008, 128, 104318.	3.0	48
42	Ab&Atilde;initio modeling of molecular IR spectra of astrophysical interest: application to CH<sub>4</sub>. Astronomy and Astrophysics, 2009, 495, 655-661.	5.1	46
43	Differential form of the collision integral for a relativistic plasma. Physical Review Letters, 1987, 59, 1817-1820.	7.8	43
44	Simulation of the Edge Plasma in Tokamaks. Physica Scripta, 2004, , 7.	2.5	42
45	QDB: a new database of plasma chemistries and reactions. Plasma Sources Science and Technology, 2017, 26, 055014.	3.1	42
46	Evidence for Vinylidene Production in the Photodissociation of the Allyl Radical. Journal of Physical Chemistry Letters, 2010, 1, 1875-1880.	4.6	40
47	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
48	Modelling of the boundary plasma of large tokamaks. Journal of Nuclear Materials, 1984, 121, 75-81.	2.7	35
49	Potential energy surface and MULTIMODE vibrational analysis of C2H3+. Journal of Chemical Physics, 2006, 125, 224306.	3.0	35
50	2D modelling of the ASDEX-Upgrade scrape-off layer and divertor plasma. Journal of Nuclear Materials, 1995, 220-222, 558-562.	2.7	34
51	The theoretical prediction of infrared spectra of <i>trans</i>- and <i>cis</i>-hydroxycarbene calculated using full dimensional <i>ab initio</i> potential energy and dipole moment surfaces. Journal of Chemical Physics, 2008, 128, 204310.	3.0	33
52	Proton affinity and enthalpy of formation of formaldehyde. International Journal of Quantum Chemistry, 2009, 109, 2393-2409.	2.0	33
53	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
54	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

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55	Progress in Integrated 2D Models for Analysis of Scrape-Off Layer Transport Physics. Contributions To Plasma Physics, 1996, 36, 105-116.	1.1	31
56	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
57	Potential energy surface and quantum dynamics study of rovibrational states for HO <sub>3</sub> (X <sup>2</sup> A <sup>3</sup> ). Physical Chemistry Chemical Physics, 2008, 10, 3150.	2.8	31
58	Analysis of cold divertor concepts for ITER. Journal of Nuclear Materials, 1995, 220-222, 1076-1080.	2.7	29
59	Ab Initio Calculation of the Photoelectron Spectra of the Hydroxycarbene Diradicals. Journal of Physical Chemistry A, 2009, 113, 7802-7809.	2.5	28
60	Accurate ab Initio Structure, Dissociation Energy, and Vibrational Spectroscopy of the F <sup>-</sup> CH <sub>4</sub> Anion Complex. Journal of Physical Chemistry A, 2008, 112, 7466-7472.	2.5	25
61	Quasiclassical trajectory calculations of the HO <sub>2</sub> + NO reaction on a global potential energy surface. Physical Chemistry Chemical Physics, 2009, 11, 4722.	2.8	25
62	Global potential energy surfaces for O(P <sub>3</sub> )+H <sub>2</sub> O(A <sub>11</sub> ) collisions. Journal of Chemical Physics, 2010, 133, 164312.	3.0	23
63	Probing the Structure of CH <sub>5</sub> <sup>+</sup> by Dissociative Charge Exchange. Journal of the American Chemical Society, 2008, 130, 3730-3731.	13.7	22
64	Sum rule constraints on Kubo-transformed correlation functions. Chemical Physics Letters, 2006, 418, 179-184.	2.6	21
65	Data on erosion and hydrogen fuel retention in Beryllium plasma-facing materials. Nuclear Materials and Energy, 2021, 27, 100994.	1.3	21
66	Two-dimensional fluid simulations of the ITER SOL plasma. Journal of Nuclear Materials, 1990, 176-177, 909-915.	2.7	20
67	Implementation into B2 of a 21-moment description for the parallel transport. Contributions To Plasma Physics, 1996, 36, 192-196.	1.1	20
68	The National Transport Code Collaboration Module Library. Computer Physics Communications, 2004, 164, 108-113.	7.5	20
69	Ro-vibrational spectra of C <sub>2</sub> H <sub>2</sub> based on variational nuclear motion calculations. Molecular Physics, 2010, 108, 1973-1990.	1.7	20
70	Quasiclassical trajectory calculations of the OH+NO <sub>2</sub> association reaction on a global potential energy surface. Journal of Chemical Physics, 2007, 127, 104310.	3.0	19
71	The Dynamics of Allyl Radical Dissociation. Journal of Physical Chemistry A, 2011, 115, 6797-6804.	2.5	19
72	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

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73	Extensions of B2 for the Simulation of ASDEX " Upgrade Scrape-off Layer Plasmas. Contributions To Plasma Physics, 1992, 32, 450-455.	1.1	18
74	Divertor tokamak operation at high densities on ASDEX Upgrade. Plasma Physics and Controlled Fusion, 1997, 39, B19-B38.	2.1	17
75	Theory and Modelling of Time Dependent Phenomena in the Plasma Edge. Contributions To Plasma Physics, 1996, 36, 150-160.	1.1	16
76	The T 1 and T 2 Representability Conditions. Advances in Chemical Physics, 2007, , 93-101.	0.3	15
77	Equilibrium clumped-isotope effects in doubly substituted isotopologues of ethane. Geochimica Et Cosmochimica Acta, 2017, 197, 14-26.	3.9	15
78	Modeling of neutral plasma in a divertor in the fluid-kinetic transition. Contributions To Plasma Physics, 1998, 38, 319-324.	1.1	14
79	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
80	Assessment of critical physical assumptions in consistent 2D plasma edge modelling. Journal of Nuclear Materials, 1992, 196-198, 466-471.	2.7	11
81	Up-down symmetry in double null divertor experiments and magnetic field topology. Nuclear Fusion, 1995, 35, 297-304.	3.5	11
82	Quasiclassical Trajectory Study of the CH3++ HD " CH2D++ H2Reaction". Journal of Physical Chemistry A, 2007, 111, 6658-6664.	2.5	11
83	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
84	TOkamak Edge Studies with A 2D Multifluid Code. Contributions To Plasma Physics, 1990, 30, 95-100.	1.1	10
85	A local interpolation method for direct classical dynamics calculations. Journal of Chemical Physics, 2001, 115, 11021-11024.	3.0	10
86	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
87	Power Balance in the ITER Plasma and Divertor. Contributions To Plasma Physics, 1996, 36, 240-244.	1.1	9
88	Nonadiabatic particle response in toroidal geometry. Physics of Fluids, 1982, 25, 1871.	1.4	8
89	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
90	Divertor design for the tokamak physics experiment. Journal of Nuclear Materials, 1995, 220-222, 698-702.	2.7	7

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91	Ab Initio Based Potential Energy Surfaces and Franck-Condon Analysis of Ionization Thresholds of Cyclic-C <sub>3</sub> H and Linear-C <sub>3</sub> H <sub>2</sub> . Journal of Physical Chemistry A, 2007, 111, 4056-4061.	2.5	7
92	Scrape-off layer modeling using coupled plasma and neutral transport codes. Journal of Nuclear Materials, 1992, 196-198, 894-898.	2.7	6
93	2 D Tokamak Edge Simulation Including Impurities. Contributions To Plasma Physics, 1988, 28, 373-378.	1.1	5
94	Diffusion of excitons in systems with non-planar geometry: theory. Chemical Physics, 2003, 288, 105-112.	1.9	5
95	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
96	Analytical potential energy surface for O+C <sub>2</sub> H <sub>2</sub> system. Chemical Physics Letters, 2013, 588, 22-26.	2.6	4
97	Scrape off layer modelling studies for SST-I. Journal of Nuclear Materials, 1999, 266-269, 726-731.	2.7	3
98	Coordinated Research Projects of the IAEA Atomic and Molecular Data Unit. , 2011, , .		3
99	B2-solps5.0: SOL transport code with drifts and currents. Contributions To Plasma Physics, 2000, 40, 328-333.	1.1	3
100	Parameter Dependence of the Edge and Divertor Plasma in Asdex Upgrade. Contributions To Plasma Physics, 1992, 32, 456-461.	1.1	2
101	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
102	Compact ignition tokamak edge and divertor modeling. , 1990, , .		1
103	Numerical Simulation of the ITER Gaseous Divertor with the B2.5 Code. Contributions To Plasma Physics, 1996, 36, 282-287.	1.1	1
104	Edge plasma analyses for KSTAR divertor design. , 0, , .		1
105	Uncertainty Quantification of theoretical atomic and molecular collisional data. Journal of Physics: Conference Series, 2015, 635, 052020.	0.4	1
106	Magnetohydrodynamic equilibrium calculations using multigrid. Lecture Notes in Mathematics, 1986, , 38-51.	0.2	0
107	Databases and coordinated research projects at the IAEA on atomic processes in plasmas. , 2012, , .		0
108	Coordinated activities on evaluation of collisional data for fusion applications. , 2013, , .		0