Oleg L Polyansky

List of Publications by Citations

80 papers	4,073 citations	36 h-index	63 g-index
86 ext. papers	4,446 ext. citations	3.5 avg, IF	5.1 L-index

#	Paper	IF	Citations
80	The ExoMol database: Molecular line lists for exoplanet and other hot atmospheres. *Journal of Molecular Spectroscopy*, **2016**, 327, 73-94	1.3	280
79	High-accuracy ab initio rotation-vibration transitions for water. *Science*, **2003**, 299, 539-42	33.3	262
78	DVR3D: a program suite for the calculation of rotation□ibration spectra of triatomic molecules. *Computer Physics Communications*, **2004**, 163, 85-116	4.2	202
77	IUPAC critical evaluation of the rotational□ibrational spectra of water vapor, Part III: Energy levels and transition wavenumbers for H216O. *Journal of Quantitative Spectroscopy and Radiative Transfer* , **2013**, 117, 29-58	2.1	185
76	ExoMol molecular line lists XXX: a complete high-accuracy line list for water. *Monthly Notices of the Royal Astronomical Society*, **2018**, 480, 2597-2608	4.3	145
75	The potential energy surface of H2 16O. *Journal of Chemical Physics*, **1996**, 105, 6490-6497	3.9	144
74	Ab initio calculation of the rotation□ibration energy levels of H3+ and its isotopomers to spectroscopic accuracy. *Journal of Chemical Physics*, **1999**, 110, 5056-5064	3.9	130
73	A global, high accuracy ab initio dipole moment surface for the electronic ground state of the water molecule. *Journal of Chemical Physics*, **2011**, 135, 034113	3.9	124
72	A spectroscopically determined potential energy surface for the ground state of H216O: A new level of accuracy. *Journal of Chemical Physics*, **1994**, 101, 7651-7657	3.9	110
71	High-Temperature Rotational Transitions of Water in Sunspot and Laboratory Spectra. *Journal of Molecular Spectroscopy*, **1997**, 186, 422-47	1.3	102
70	The near infrared, visible, and near ultraviolet overtone spectrum of water. *Journal of Chemical Physics*, **1999**, 111, 2444-2450	3.9	101
69	Ab initio global potential, dipole, adiabatic, and relativistic correction surfaces for the HCN□HNC system. *Journal of Chemical Physics*, **2001**, 115, 3706-3718	3.9	96
68	Total internal partition sums for 166 isotopologues of 51 molecules important in planetary atmospheres: Application to HITRAN2016 and beyond. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2017**, 203, 70-87	2.1	94
67	High-Accuracy CO(2) Line Intensities Determined from Theory and Experiment. *Physical Review Letters*, **2015**, 114, 243001	7.4	91
66	Vibration-rotation levels of water beyond the Born-Oppenheimer approximation. *Chemical Physics Letters*, **1996**, 260, 381-387	2.5	89
65	Spectroscopically determined potential energy surface of H216O up to 25 000 cm□1. *Journal of Chemical Physics*, **2003**, 118, 2124-2129	3.9	87
64	A room temperature CO2 line list with ab initio computed intensities. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2016**, 177, 31-42	2.1	84

63	Precision measurements and computations of transition energies in rotationally cold triatomic hydrogen ions up to the midvisible spectral range. *Physical Review Letters*, **2012**, 108, 023002	7.4	80
62	Estimation of Lamb-shift effects for molecules: Application to the rotation-vibration spectra of water. *Physical Review A*, **2001**, 63,	2.6	76
61	A new ab initio ground-state dipole moment surface for the water molecule. *Journal of Chemical Physics*, **2008**, 128, 044304	3.9	75
60	First-principles prediction and partial characterization of the vibrational states of water up to dissociation. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2010**, 111, 1043-1064	2.1	70
59	Calibration-quality adiabatic potential energy surfaces for H3(+) and its isotopologues. *Journal of Chemical Physics*, **2012**, 136, 184303	3.9	65
58	Monodromy in the water molecule. *Chemical Physics Letters*, **2005**, 414, 193-197	2.5	63
57	Calculation of rotation-vibration energy levels of the water molecule with near-experimental accuracy based on an ab initio potential energy surface. *Journal of Physical Chemistry A*, **2013**, 117, 9633-43	2.8	60
56	[ITAL]K[/ITAL]-Band Spectrum of Water in Sunspots. *Astrophysical Journal*, **1997**, 489, L205-L208	4.7	55
55	Accurate bond dissociation energy of water determined by triple-resonance vibrational spectroscopy and ab initio calculations. *Chemical Physics Letters*, **2013**, 568-569, 14-20	2.5	54
54	Relativistic correction to the potential energy surface and vibration-rotation levels of water. *Chemical Physics Letters*, **1998**, 293, 317-323	2.5	54
53	State-selective spectroscopy of water up to its first dissociation limit. *Journal of Chemical Physics*, **2009**, 131, 221105	3.9	51
52	Water line lists close to experimental accuracy using a spectroscopically determined potential energy surface for H2(16)O, H2(17)O, and H2(18)O. *Journal of Chemical Physics*, **2008**, 128, 224306	3.9	51
51	The Emission Spectrum of Hot Water in the Region between 370 and 930 cm1. *Journal of Molecular Spectroscopy*, **1996**, 176, 305-315	1.3	50
50	A global potential energy surface for the H3+ molecule. *Chemical Physics Letters*, **1997**, 273, 107-114	2.5	44
49	Opacity Data for HCN and HNC from a New Ab Initio Line List. *Astrophysical Journal*, **2002**, 578, 657-663	4.7	43
48	An accurate, global, ab initio potential energy surface for the H+ 3 molecule. *Molecular Physics*, **2000**, 98, 261-273	1.7	41
47	New Assignments for the Infrared Spectrum of H3+. *Journal of Molecular Spectroscopy*, **1997**, 181, 142-150	1.3	39
46	Room temperature line lists for CO2 symmetric isotopologues with ab initio computed intensities. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2017**, 189, 267-280	2.1	37

45	Vibrationally and rotationally nonadiabatic calculations on H3+ using coordinate-dependent vibrational and rotational masses. *Physical Review A*, **2013**, 88,	2.6	36
44	Approaching the full set of energy levels of water. *Journal of Chemical Physics*, **2007**, 126, 241101	3.9	36
43	Spectroscopically determined Born□Oppenheimer and adiabatic surfaces for H3+, H2D+, D2H+, and D3+. *Journal of Chemical Physics*, **1995**, 103, 10433-10438	3.9	36
42	Two-electron relativistic corrections to the potential energy surface and vibration□otation levels of water. *Chemical Physics Letters*, **2001**, 344, 413-420	2.5	35
41	Global spectroscopy of the water monomer. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2012**, 370, 2728-48	3	33
40	Spectroscopy of H3+ based on a new high-accuracy global potential energy surface. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2012**, 370, 5014-27	3	32
39	Ab initio rotation-vibration energy levels of triatomics to spectroscopic accuracy. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2002**, 58, 663-72	4.4	32
38	Asymmetric adiabatic correction to the rotation□ibration levels of H2D+ and D2H+. *Journal of Chemical Physics*, **1995**, 102, 9322-9326	3.9	30
37	Ab initio rovibrational spectroscopy of hydrogen sulfide. *Journal of Chemical Physics*, **2001**, 115, 1229-1242	3.9	29
36	Accurate line intensities for water transitions in the infrared: Comparison of theory and experiment. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2017**, 203, 88-102	2.1	28
35	Ab initio rotation-vibration spectra of HCN and HNC. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2002**, 58, 673-90	4.4	28
34	Room temperature linelists for CO2 asymmetric isotopologues with ab initio computed intensities. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2017**, 203, 265-281	2.1	27
33	First-principles rotation□ibration spectrum of water above dissociation. *Chemical Physics Letters*, **2011**, 507, 48-51	2.5	27
32	Collisionally assisted spectroscopy of water from 27,000 to 34,000 cm(-1). *Journal of Physical Chemistry A*, **2008**, 112, 10539-45	2.8	27
31	ExoMol molecular line lists □XX. A comprehensive line list for H3+. *Monthly Notices of the Royal Astronomical Society*, **2017**, 468, 1717-1725	4.3	25
30	Calculation of rotation-vibration energy levels of the ammonia molecule based on an ab initio potential energy surface. *Journal of Molecular Spectroscopy*, **2016**, 327, 21-30	1.3	23
29	Improved potential energy surface and spectral assignments for ammonia in the near-infrared region. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2018**, 219, 199-212	2.1	21
28	High-accuracy water potential energy surface for the calculation of infrared spectra. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2018**, 376,	3	20

27	QED correction for H3+. *Physical Review A*, **2014**, 89,	2.6	18
26	A highly accurate dipole moment surface for the ground electronic state of water vapour for spectra extending into the ultraviolet. *Journal of Chemical Physics*, **2018**, 149, 084307	3.9	17
25	Communication: Visible line intensities of the triatomic hydrogen ion from experiment and theory. *Journal of Chemical Physics*, **2014**, 141, 241104	3.9	15
24	Variational calculation of highly excited rovibrational energy levels of H2O2. *Journal of Physical Chemistry A*, **2013**, 117, 7367-77	2.8	14
23	High-accuracy calculations of the rotation-vibration spectrum of ${{rm{H}}}_{3}^{+}$. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2017**, 50, 232001	1.3	13
22	Potential energy surface, dipole moment surface and the intensity calculations for the 10 μm, 5 μm and 3 μm bands of ozone. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2018**, 210, 127-135	2.1	12
21	Calculations of rotation□ibration states with the z axis perpendicular to the plane: High accuracy results for H3+. *Journal of Chemical Physics*, **2002**, 116, 7564-7573	3.9	12
20	The W2020 Database of Validated Rovibrational Experimental Transitions and Empirical Energy Levels of Water Isotopologues. II. H217O and H218O with an Update to H216O. *Journal of Physical and Chemical Reference Data*, **2020**, 49, 043103	4.3	12
19	A global potential energy surface for H3+. *Molecular Physics*, **2019**, 117, 1663-1672	1.7	11
18	W2020: A Database of Validated Rovibrational Experimental Transitions and Empirical Energy Levels of H216O. *Journal of Physical and Chemical Reference Data*, **2020**, 49, 033101	4.3	10
17	Absorption spectra of ammonia near 1 μm. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2017**, 203, 392-397	2.1	10
16	On the determination of potential energy surfaces of spectroscopic accuracy. *Computational and Theoretical Chemistry*, **1995**, 341, 133-140		9
15	Analysis of the red and green optical absorption spectrum of gas phase ammonia. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2018**, 209, 224-231	2.1	8
14	A semi-empirical potential energy surface and line list for H₂¹⁶O extending into the near-ultraviolet. *Atmospheric Chemistry and Physics*, **2020**, 20, 10015-10027	6.8	8
13	Calculated line lists for H216O and H218O with extensive comparisons to theoretical and experimental sources including the HITRAN2016 database. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2020**, 241, 106711	2.1	8
12	High Accuracy ab Initio Calculations of Rotational-Vibrational Levels of the HCN/HNC System. *Journal of Physical Chemistry A*, **2018**, 122, 1326-1343	2.8	7
11	Use of the complete basis set limit for computing highly accurate ab initio dipole moments. *Journal of Chemical Physics*, **2020**, 152, 024105	3.9	6
10	A new spectroscopically-determined potential energy surface and ab initio dipole moment surface for high accuracy HCN intensity calculations. *Journal of Molecular Spectroscopy*, **2018**, 353, 40-53	1.3	6

9	Saddle point localization of molecular wavefunctions. *Scientific Reports*, **2016**, 6, 33068	4.9	5
8	Ab initio calculation of the ro-vibrational spectrum of H2F+. *Journal of Molecular Spectroscopy*, **2015**, 316, 38-44	1.3	4
7	Synthesis of ab initio and effective Hamiltonian line lists for ozone. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2021**, 269, 107651	2.1	3
6	Absolute 13C/12C isotope amount ratio for Vienna PeeDee Belemnite from infrared absorption spectroscopy. *Nature Physics*, **2021**, 17, 889-893	16.2	2
5	Variational analysis of HF dimer tunneling rotational spectra using an ab initio potential energy surface. *Journal of Molecular Spectroscopy*, **2021**, 379, 111481	1.3	1
4	An experimentally-accurate and complete room-temperature infrared HCN line-list for the HITRAN database. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2021**, 270, 107666	2.1	1
3	Determination of quantum labels based on projections of the total angular momentum on the molecule-fixed axis. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2021**, 270, 107716	2.1	1
2	The spectrum of ammonia near 0.793 μm. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2021**, 273, 107838	2.1	1
1	Highly accurate HF dimer ab initio potential energy surface.. *Journal of Chemical Physics*, **2022**, 156, 164305	3.9	