Sergei N Yurchenko

List of Publications by Citations

249 papers	8,709 citations	48 h-index	82 g-index
270 ext. papers	10,502 ext. citations	3.5 avg, IF	6.65 L-index

#	Paper	IF	Citations
249	Graphene nanostructures as tunable storage media for molecular hydrogen. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 10439-44	11.5	487
248	ExoMol: molecular line lists for exoplanet and other atmospheres. *Monthly Notices of the Royal Astronomical Society*, **2012**, 425, 21-33	4.3	300
247	The ExoMol database: Molecular line lists for exoplanet and other hot atmospheres. *Journal of Molecular Spectroscopy*, **2016**, 327, 73-94	1.3	280
246	A variationally computed line list for hot NH3. *Monthly Notices of the Royal Astronomical Society*, **2011**, 413, 1828-1834	4.3	241
245	ExoMol line lists IV. The rotation–vibration spectrum of methane up to 1500 K. *Monthly Notices of the Royal Astronomical Society*, **2014**, 440, 1649-1661	4.3	235
244	Theoretical ROVibrational Energies (TROVE): A robust numerical approach to the calculation of rovibrational energies for polyatomic molecules. *Journal of Molecular Spectroscopy*, **2007**, 245, 126-140	1.3	223
243	TAU-REX I: A NEXT GENERATION RETRIEVAL CODE FOR EXOPLANETARY ATMOSPHERES. *Astrophysical Journal*, **2015**, 802, 107	4.7	161
242	DETECTION OF AN ATMOSPHERE AROUND THE SUPER-EARTH 55 CANCRI E. *Astrophysical Journal*, **2016**, 820, 99	4.7	156
241	A chemical survey of exoplanets with ARIEL. *Experimental Astronomy*, **2018**, 46, 135-209	1.3	148
240	A variationally computed T = 300 K line list for NH3. *Journal of Physical Chemistry A*, **2009**, 113, 11845-55	2.8	147
239	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
238	A Population Study of Gaseous Exoplanets. *Astronomical Journal*, **2018**, 155, 156	4.9	144
237	Water vapour in the atmosphere of the habitable-zone eight-Earth-mass planet K2-18 b. *Nature Astronomy*, **2019**, 3, 1086-1091	12.1	127
236	${mathcal{T}}$-REx. II. RETRIEVAL OF EMISSION SPECTRA. *Astrophysical Journal*, **2015**, 813, 13	4.7	104
235	The discovery of a very cool, very nearby brown dwarf in the Galactic plane. *Monthly Notices of the Royal Astronomical Society: Letters*, **2010**, 408, L56-L60	4.3	104
234	Probing the extreme planetary atmosphere of WASP-12b. *Icarus*, **2013**, 225, 432-445	3.8	102
233	ExoMol line lists III. An improved hot rotation-vibration line list for HCN and HNC. *Monthly Notices of the Royal Astronomical Society*, **2014**, 437, 1828-1835	4.3	101

232	Duo: A general program for calculating spectra of diatomic molecules. *Computer Physics Communications*, **2016**, 202, 262-275	4.2	98
231	METHANE IN THE ATMOSPHERE OF THE TRANSITING HOT NEPTUNE GJ436B?. *Astrophysical Journal*, **2011**, 731, 16	4.7	96
230	The HITRAN2020 molecular spectroscopic database. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2021**, 277, 107949	2.1	96
229	An ab initio study of the CH3I photodissociation. I. Potential energy surfaces. *Journal of Chemical Physics*, **2007**, 126, 234102	3.9	95
228	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
227	Laser-induced interference, focusing, and diffraction of rescattering molecular photoelectrons. *Physical Review Letters*, **2004**, 93, 223003	7.4	90
226	Temperature-dependent molecular absorption cross sections for exoplanets and other atmospheres. *Icarus*, **2013**, 226, 1673-1677	3.8	87
225	ExoMol molecular line lists XXXIII. The spectrum of Titanium Oxide. *Monthly Notices of the Royal Astronomical Society*, **2019**, 488, 2836-2854	4.3	84
224	Spectrum of hot methane in astronomical objects using a comprehensive computed line list. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 9379-83	11.5	83
223	Structure-based sampling and self-correcting machine learning for accurate calculations of potential energy surfaces and vibrational levels. *Journal of Chemical Physics*, **2017**, 146, 244108	3.9	82
222	EChO. *Experimental Astronomy*, **2012**, 34, 311-353	1.3	82
221	ExoMol line lists XVIII. The high-temperature spectrum of VO. *Monthly Notices of the Royal Astronomical Society*, **2016**, 463, 771-793	4.3	80
220	EXOCROSS: a general program for generating spectra from molecular line lists. *Astronomy and Astrophysics*, **2018**, 614, A131	5.1	78
219	ExoMol line lists VII. The rotation–vibration spectrum of phosphine up to 1500 K. *Monthly Notices of the Royal Astronomical Society*, **2015**, 446, 2337-2347	4.3	75
218	ExoMol line lists II. The ro-vibrational spectrum of SiO. *Monthly Notices of the Royal Astronomical Society*, **2013**, 434, 1469-1475	4.3	75
217	Towards efficient refinement of molecular potential energy surfaces: Ammonia as a case study. *Journal of Molecular Spectroscopy*, **2011**, 268, 123-129	1.3	71
216	Vibrational transition moments of CH4 from first principles. *Journal of Molecular Spectroscopy*, **2013**, 291, 69-76	1.3	69
215	A high accuracy computed line list for the HDO molecule. *Monthly Notices of the Royal Astronomical Society*, **2010**, 402, 492-496	4.3	67

214	Vibrational energies for NH3 based on high level ab initio potential energy surfaces. *Journal of Chemical Physics*, **2002**, 117, 11265-11276	3.9	67
213	ExoMol molecular line lists □X. The spectrum of AlO. *Monthly Notices of the Royal Astronomical Society*, **2015**, 449, 3613-3619	4.3	66
212	Potential-energy surface for the electronic ground state of NH3 up to 20,000 cm-1 above equilibrium. *Journal of Chemical Physics*, **2005**, 123, 134308	3.9	66
211	BLIND EXTRACTION OF AN EXOPLANETARY SPECTRUM THROUGH INDEPENDENT COMPONENT ANALYSIS. *Astrophysical Journal*, **2013**, 766, 7	4.7	61
210	MARVEL analysis of the measured high-resolution spectra of 14NH3. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2015**, 161, 117-130	2.1	60
209	ExoMol line lists - I. The rovibrational spectrum of BeH, MgH and CaH in theX 2□state. *Monthly Notices of the Royal Astronomical Society*, **2012**, 425, 34-43	4.3	59
208	Automatic differentiation method for numerical construction of the rotational-vibrational Hamiltonian as a power series in the curvilinear internal coordinates using the Eckart frame. *Journal of Chemical Physics*, **2015**, 143, 014105	3.9	57
207	Laboratory spectra of hot molecules: Data needs for hot super-Earth exoplanets. *Molecular Astrophysics*, **2017**, 8, 1-18	1.7	55
206	The 2020 release of the ExoMol database: Molecular line lists for exoplanet and other hot atmospheres. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2020**, 255, 107228	2.1	54
205	ExoMol molecular line lists □XVI. The rotation□ibration spectrum of hot H2S. *Monthly Notices of the Royal Astronomical Society*, **2016**, 460, 4063-4074	4.3	54
204	Rotation□ibration motion of pyramidal XY3 molecules described in the Eckart frame: Theory and application to NH3. *Molecular Physics*, **2005**, 103, 359-378	1.7	52
203	ExoMol line list □XXI. Nitric Oxide (NO). *Monthly Notices of the Royal Astronomical Society*, **2017**, 470, 882-897	4.3	51
202	A hybrid line list for CH and hot methane continuum. *Astronomy and Astrophysics*, **2017**, 605,	5.1	49
201	Potential parameters of PH3 obtained by simultaneous fitting of ab initio data and experimental vibrational band origins. *Chemical Physics*, **2003**, 290, 59-67	2.3	48
200	ExoMol molecular line lists □XIV. The rotation□ibration spectrum of hot SO2. *Monthly Notices of the Royal Astronomical Society*, **2016**, 459, 3890-3899	4.3	47
199	Re-analysis of ammonia spectra: Updating the HITRAN 14NH3 database. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2013**, 130, 260-272	2.1	47
198	Theab initiocalculation of spectra of open shell diatomic molecules. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2016**, 49, 102001	1.3	47
197	Symmetry-Adapted Ro-vibrational Basis Functions for Variational Nuclear Motion Calculations: TROVE Approach. *Journal of Chemical Theory and Computation*, **2017**, 13, 4368-4381	6.4	45

196	Methane and ammonia in the near-infrared spectra of late-T dwarfs. *Monthly Notices of the Royal Astronomical Society*, **2015**, 450, 454-480	4.3	45
195	High temperature partition functions and thermodynamic data for ammonia and phosphine. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2014**, 142, 66-74	2.1	44
194	A new "spectroscopic" potential energy surface for formaldehyde in its ground electronic state. *Journal of Chemical Physics*, **2011**, 134, 244307	3.9	44
193	Ab initio dipole moment and theoretical rovibrational intensities in the electronic ground state of PH3. *Journal of Molecular Spectroscopy*, **2006**, 239, 71-87	1.3	44
192	ExoMol line lists VIII. A variationally computed line list for hot formaldehyde. *Monthly Notices of the Royal Astronomical Society*, **2015**, 448, 1704-1714	4.3	42
191	A computed room temperature line list for phosphine. *Journal of Molecular Spectroscopy*, **2013**, 288, 28-37	1.3	42
190	Lightning chemistry on Earth-like exoplanets. *Monthly Notices of the Royal Astronomical Society*, **2017**, 470, 187-196	4.3	41
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185	Optimized semiempirical potential energy surface for H2 16O up to 26000 cm−1. *Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)*, **2011**, 110, 160-166	0.7	37
184	EXPERIMENTAL ENERGY LEVELS AND PARTITION FUNCTION OF THE 12 C 2 MOLECULE. *Astrophysical Journal, Supplement Series*, **2016**, 224, 44	8	37
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182	The ExoMol Atlas of Molecular Opacities. *Atoms*, **2018**, 6, 26	2.1	36
181	Terahertz spectroscopy of hydrogen sulfide. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2013**, 130, 341-351	2.1	36
180	Hydrogen storage in zeolite imidazolate frameworks. A multiscale theoretical investigation. *International Journal of Hydrogen Energy*, **2011**, 36, 6005-6013	6.7	36
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178	Study of the electronic and rovibronic structure of the X □, A □ and B □ states of AlO. *Journal of Chemical Physics*, **2014**, 141, 144312	3.9	35
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171	Global spectroscopy of the water monomer. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2012**, 370, 2728-48	3	33
170	Spectroscopic line parameters of NO, NO2, and N2O for the HITEMP database. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2019**, 232, 35-53	2.1	32
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168	Theoretical evidence for the formation of rotational energy level clusters in the vibrational ground state of PH3. *Physical Chemistry Chemical Physics*, **2005**, 7, 573-82	3.6	32
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164	ExoMol molecular line lists □XXVII. Spectra of C2H4. *Monthly Notices of the Royal Astronomical Society*, **2018**, 478, 3220-3232	4.3	29
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161	Thermal averaging of the indirect nuclear spin-spin coupling constants of ammonia: the importance of the large amplitude inversion mode. *Journal of Chemical Physics*, **2010**, 132, 114305	3.9	28

160	An ab initio calculation of the vibrational energies and transition moments of HSOH. *Journal of Molecular Spectroscopy*, **2009**, 257, 57-65	1.3	28
159	A variationally calculated room temperature line-list for H 2 O 2. *Journal of Molecular Spectroscopy*, **2015**, 318, 84-90	1.3	27
158	ExoMol molecular line lists XVII. The rotation–vibration spectrum of hot SO3. *Monthly Notices of the Royal Astronomical Society*, **2016**, 462, 4300-4313	4.3	26
157	A global potential energy surface and dipole moment surface for silane. *Journal of Chemical Physics*, **2015**, 143, 244317	3.9	26
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155	Vibrational energies of PH3 calculated variationally at the complete basis set limit. *Journal of Chemical Physics*, **2008**, 129, 044309	3.9	26
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153	ExoMol line lists XXIV: a new hot line list for silicon monohydride, SiH. *Monthly Notices of the Royal Astronomical Society*, **2018**, 473, 5324-5333	4.3	26
152	ExoMol molecular line lists XXIII. Spectra of PO and PS. *Monthly Notices of the Royal Astronomical Society*, **2017**, 472, 3648-3658	4.3	25
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145	An ab initio variationally computed room-temperature line list for (32)S(16)O3. *Physical Chemistry Chemical Physics*, **2013**, 15, 10118-25	3.6	23
144	High-level ab initio potential energy surfaces and vibrational energies of H2CS. *Journal of Chemical Physics*, **2011**, 135, 074302	3.9	23
143	Five carbon- and nitrogen-bearing species in a hot giant planet's atmosphere. *Nature*, **2021**, 592, 205-208	50.4	23

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139	The ExoMol pressure broadening diet: H2 and He line-broadening parameters. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2017**, 203, 490-495	2.1	21
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127	High-resolution absorption measurements of NH3 at high temperatures: 5002100 cm1. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2015**, 167, 126-134	2.1	18
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108	Determination of glyphosate in surface water with high organic matter content. *Environmental Science and Pollution Research*, **2017**, 24, 7880-7888	5.1	13
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93	A weak spectral signature of water vapour in the atmosphere of HD 179949 b at high spectral resolution in the L band. *Monthly Notices of the Royal Astronomical Society*, **2020**, 494, 108-119	4.3	10
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