Nikolaj F Stepanov

List of Publications by Year
in descending order

101 papers	1,006 citations	471061 17 h-index	525886 27 g-index
103 all docs	103 docs citations	103 times ranked	687 citing authors

#	Article	IF	Citations
1	Arâ€“I2interactions: The models based on the diatomicsâ€inâ€molecule approach. Journal of Chemical Physics, 1996, 104, 9913-9925.	1.2	88
2	Numerical-Analytic Implementation of the Higher-Order Canonical Van Vleck Perturbation Theory for the Interpretation of Medium-Sized Molecule Vibrational Spectra. Journal of Physical Chemistry A, 2012, 116, 3691-3709.	1.1	69
3	Theoretical Study of Structure and Electronic Absorption Spectra of Some Schiff Bases and Their Zinc Complexes. Inorganic Chemistry, 2009, 48, 11123-11130.	1.9	56
4	Vibration-rotation problem for triatomic molecules with two large-amplitude coordinates. Journal of Molecular Spectroscopy, 1977, 67, 265-282.	0.4	40
5	Simulation of structured 4T1â†'6A1 emission bands of Mn2+ impurity in Zn2SiO4: A first-principle methodology. Journal of Luminescence, 2012, 132, 2143-2150.	1.5	39
6	Small Charged Water Clusters:â€‰ Cations. Journal of Physical Chemistry A, 1999, 103, 3285-3288.	1.1	38
7	Anharmonic Vibrational Analysis of the Gas-Phase Infrared Spectrum of 1,1-Difluoroethylene Using the Operator Van Vleck Canonical Perturbation Theory. Journal of Physical Chemistry A, 2013, 117, 3041-3056.	1.1	30
8	Environmental Broadening of the CTTS Bands: The Hexaammineruthenium(II) Complex in Aqueous Solution. Journal of Physical Chemistry A, 2010, 114, 12804-12812.	1.1	26
9	ArHF vibrational predissociation dynamics using the diatomics-in-molecule potential energy surface. Journal of Chemical Physics, 1999, 111, 2470-2477.	1.2	25
10	Diatomics-in-molecules description of the Rgâ€“Hal2 rare gasâ€“halogen van der Waals complexes with applications to Heâ€“Cl2. Journal of Chemical Physics, 1997, 106, 4575-4588.	1.2	23
11	Two-centre model potential energy calculations for the 2Î£ and 2Î states of Li+2, Na+2, K+2, Rb+2 and Cs+2. Chemical Physics Letters, 1979, 60, 421-426.	1.2	22
12	Molecular structure of the boron(III) oxide molecule in the SCF approximation. Journal of Molecular Structure, 1980, 68, 199-202.	1.8	21
13	Interaction potentials and fragmentation dynamics of the Neâ‹¯Br2complex in the ground and electronically excited states. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 3229-3236.	1.7	21
14	Errors in molecular integrals: An influence onRHF energy values. International Journal of Quantum Chemistry, 1977, 11, 1-15.	1.0	18
15	First-order intermolecular diatomics-in-molecule potentials. Potential energy surfaces, spectra, and fragmentation dynamics of the Neâ‹¯Cl2 complex. Journal of Chemical Physics, 1997, 106, 10134-10144.	1.2	18
16	Small Charged Water Clusters:Â Anions. Journal of Physical Chemistry A, 1999, 103, 10975-10980.	1.1	17
17	Simulating the structureless emission bands of Mn2+ ions in ZnCO3 and CaCO3 matrices by means of quantum chemistry. Russian Journal of Physical Chemistry A, 2013, 87, 245-251.	0.1	17
18	The potential surface of the ground state and the force field of the B2O2 molecule in the SCF approximation. Journal of Structural Chemistry, 1983, 24, 252-254.	0.3	16

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19	Structure and interaction energies of the Arâ€¦Cl2 complex. Application of first-order intermolecular potentials. Chemical Physics Letters, 1996, 261, 591-596.	1.2	15
20	Some aspects of scaling the molecular quantum mechanical force field. Journal of Molecular Structure, 1996, 376, 363-368.	1.8	15
21	Electron hydration: interface shells. Chemical Physics Letters, 2001, 344, 619-624.	1.2	15
22	Nonempirical Description of the Atmospherically Important Anionic Species. I. Water Cluster Anions. Structural Chemistry, 2004, 15, 65-70.	1.0	15
23	Vibrational predissociation of ArHF: a test of global semiempirical potential energy surfaces. Physical Chemistry Chemical Physics, 2002, 4, 4992-4998.	1.3	14
24	Vibrationâ€”rotation hamiltonian for nonrigid triatomic molecules with diatomic rigid core. Chemical Physics, 1978, 31, 413-423.	0.9	13
25	Diatomics-in-molecules study of LiOH. International Journal of Quantum Chemistry, 1979, 15, 49-56.	1.0	13
26	Molecular structure of acetyldeyiethylphosphine, MeC(O)PMe2. Journal of Molecular Structure, 1977, 37, 251-259.	1.8	12
27	Vibrational spectra and conformational analysis of five chlorosubstituted buta-1,3-dienes. Journal of Molecular Structure, 1978, 49, 17-27.	1.8	12
28	Electronic structure and electronic absorption spectra of molybdenum and tungsten oxotetrachlorides. Theoretica Chimica Acta, 1980, 56, 297-306.	0.9	12
29	The Kirkwoodâ€“Buckingham variational method and the boundary value problems for the molecular SchrÃ¶dinger equation. Journal of Mathematical Physics, 1997, 38, 5626-5633.	0.5	12
30	Ab Initio Vibrational Analysis of Cyclopropene, Its Fluoro Derivatives, and Their Deutero Analogues. Journal of Physical Chemistry A, 1998, 102, 2363-2371.	1.1	12
31	Stationary states and dissociation of H3O radical in water clusters. Russian Journal of Physical Chemistry A, 2009, 83, 798-808.	0.1	12
32	Kinematic models of a force field. Journal of Molecular Structure, 1972, 12, 289-297.	1.8	11
33	Diatomics-in-molecules study of alkali hydroxides. Journal of Molecular Structure, 1980, 67, 81-88.	1.8	11
34	Advantages of scaled quantum mechanical molecular force fields. Journal of Molecular Structure, 1995, 348, 413-416.	1.8	11
35	DIM potential energy surfaces for excited states of H3. Molecular Physics, 1980, 41, 377-382.	0.8	10
36	Molecular mechanism of hydrogen bromide addition to olefins. Tetrahedron, 1982, 38, 2585-2589.	1.0	10

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37	Importance of correlation in LiBO. Theoretica Chimica Acta, 1985, 67, 287-292.	0.9	9
38	On the use of restricted CI for correlation energy calculations: Application to BH. Chemical Physics Letters, 1985, 115, 241-244.	1.2	9
39	Hydrated electron: Nonempirical cluster approach. International Journal of Quantum Chemistry, 2002, 88, 496-506.	1.0	9
40	Convergence problems in the solution of SCF equations. International Journal of Quantum Chemistry, 1974, 8, 107-117.	1.0	8
41	Approximate phaseâ€space transport theory for vibrational predissociation. Journal of Chemical Physics, 1993, 98, 5486-5498.	1.2	8
42	Half- and full-collision VT energy transfer in the Heî—¸Br2(B) system. Chemical Physics Letters, 1997, 269, 448-454.	1.2	8
43	Classical vibrational predissociation dynamics: The effects of phase-space bifurcations. Journal of Chemical Physics, 1998, 108, 6282-6290.	1.2	7
44	When and why Hund's cases arise. Journal of Molecular Spectroscopy, 1974, 52, 277-286.	0.4	6
45	A new derivation for the Tellerâ€”Redlich isotopic product rule. Vibrational Spectroscopy, 1994, 7, 191-196.	1.2	6
46	Theoretical study of VRT energy transfer in Ne+I2(B) collisions using a spectroscopic interaction potential. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 2307-2313.	1.7	6
47	Comparative analysis of the state of lithium and sodium atoms in water clusters. Russian Journal of Physical Chemistry A, 2009, 83, 1134-1144.	0.1	6
48	A quantum-chemical and gas phase electron diffraction study of the structure of formylphosphine and acetyldimethylphosphine. Russian Journal of Physical Chemistry A, 2010, 84, 1745-1751.	0.1	6
49	Electronic structure and one-electron properties of the MoO2Cl2 molecule. Electronic spectra of the MoO2Cl2, MoO2Br2 and WO2Br2 molecules. Theoretica Chimica Acta, 1982, 61, 369-377.	0.9	5
50	Diatomics-in-molecules studies of the Li + H2O interaction. Computational and Theoretical Chemistry, 1983, 104, 403-409.	1.5	5
51	Some Aspects of the Implementation of Scaling Quantum Mechanical Molecular Force Fields. Structural Chemistry, 2004, 15, 95-101.	1.0	5
52	The determination of the equilibrium geometry of a molecule with the use of microwave data and theoretical rotational-vibrational interaction constants. Russian Journal of Physical Chemistry A, 2006, 80, 1448-1455.	0.1	5
53	Scale factors as effective parameters for correcting nonempirical force fields. Russian Journal of Physical Chemistry A, 2007, 81, 585-592.	0.1	5
54	The applicability of TD-DFT methods to calculations of the electronic absorption spectrum of hexaamminoruthenium(II) in aqueous solution. Russian Journal of Physical Chemistry A, 2010, 84, 39-43.	0.1	5

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55	Nuclear charge changes: Influence on the energy of highly symmetrical molecules. Chemical Physics Letters, 1977, 45, 589-591.	1.2	4
56	The extreme values of mean-square amplitudes of molecular vibrations. Journal of Molecular Structure, 1978, 43, 101-108.	1.8	4
57	CNDO/2 calculations of intermolecular interactions in chlorine-ethylene and bromine-ethylene systems. Advances in Molecular Relaxation and Interaction Processes, 1978, 12, 325-332.	0.6	4
58	On diatomic state mixing and treatment of overlap in the diatomics-in-molecules theory. Chemical Physics Letters, 1979, 63, 396-400.	1.2	4
59	Calculation of the potential curves of the low-lying electronic states of LiBe and LiBe+ in a mixed orbital basis by the SCF method. Journal of Structural Chemistry, 1983, 24, 321-323.	0.3	4
60	The vibrational predissociation lifetime of the Heâ€¦N+2 (X, Î½ = 1) complex. Chemical Physics Letters, 1994, 220, 93-96.	1.2	4
61	Possible transformations of the ozone molecule in the presence of water associates. Russian Journal of Physical Chemistry A, 2006, 80, 106-114.	0.1	4
62	Hybrid Ab initio/EFP approach for calculating dâ€d absorption spectrum of hexaammineruthenium(II) ion in aqueous solutions. International Journal of Quantum Chemistry, 2008, 108, 2711-2718.	1.0	4
63	The conformational analysis of 2,3,4,5-tetrachloro-trans-hexa-1,3,5-triene. Journal of Molecular Structure, 1975, 29, 329-334.	1.8	3
64	Concerning the physical solution of the inverse vibrational problem. Journal of Molecular Structure, 1975, 27, 423-431.	1.8	3
65	Electron spectra and one-electron properties of the WOCl 4 , WSCl 4 and WOBr 4 molecules. Chemical Physics, 1980, 53, 63-69.	0.9	3
66	Ab initiofinite-field transition moment calculations. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, 5275-5280.	0.6	3
67	Interpreting the vibrational spectra of uracil molecules and their deuterated isotopomers using a scaled quantum-chemical quadratic force field. Russian Journal of Physical Chemistry A, 2012, 86, 1855-1861.	0.1	3
68	A theoretical study of the molecule of boric oxide B2O3. Journal of Structural Chemistry, 1981, 22, 21-28.	0.3	2
69	Influence of the choice of the adiabatic approximation and nonadiabatic effects on molecular structure. Journal of Structural Chemistry, 1983, 24, 17-24.	0.3	2
70	Fragment-localized analysis of the multiconfigurational wavefunctions. Chemical Physics, 1990, 148, 309-314.	0.9	2
71	Effect of scaling of a quantum mechanical force field on the frequencies and forms of molecular vibrations. Journal of Structural Chemistry, 1998, 39, 169-174.	0.3	2
72	Nitrite ion formation: Nonempirical simulation in terms of cluster model. International Journal of Quantum Chemistry, 2004, 100, 460-468.	1.0	2

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73	<title>Ultraviolet-light absorption and electron localization by ozone in the presence of water: nonempirical consideration</title>. , 2004, , .		2
74	Properties of methanol bound to a defect of zeolitic structure. International Journal of Quantum Chemistry, 2005, 104, 214-222.	1.0	2
75	On the kashiwagi-sasaki generalization of the lÃ¶wdin orthogonalization and the inverse vibrational problem. International Journal of Quantum Chemistry, 1977, 12, 317-326.	1.0	1
76	Possible generalization of the optimized diatomics-in molecules theory: Further studies of the diatomic state mixing parameter adjustment. International Journal of Quantum Chemistry, 1980, 17, 679-687.	1.0	1
77	A study of the potential surface of the groud state of HCN by the method of diatomic fragments in molecules. Journal of Structural Chemistry, 1981, 22, 147-152.	0.3	1
78	Unitary transformations with the unitary operators depending on projection operators. International Journal of Quantum Chemistry, 1981, 19, 793-803.	1.0	1
79	A study of the potential surface of LiOB by the method of diatomic fragments in molecules. Journal of Structural Chemistry, 1983, 24, 339-343.	0.3	1
80	Approximate treatment of the phase-space bottlenecks for vibrational predissociation. Journal of Physics B: Atomic, Molecular and Optical Physics, 1991, 24, L545-L549.	0.6	1
81	Approximate Quantal Calculations on the Predissociative Lifetimes of the Neâ€¦Hal₂(X,v) (Hal = Cl,Br,I) Van Der Waals Complexes. Spectroscopy Letters, 1992, 25, 189-200.	0.5	1
82	Three-dimensional quantum calculations on the He...Br2 (B) predissociative linewidths. , 1994, 2205, 178.		1
83	Calculations of spectra and dynamics of rare-gas halogen molecule complexes using the semi-empirical potential energy surfaces. , 1997, , .		1
84	Nonempirical estimation of the ionization conditions of water and amorphous ice. Russian Journal of Physical Chemistry A, 2007, 81, 941-948.	0.1	1
85	Rate constants of atomic hydrogen formation in H3O+(H2O) n + e â†' H + (H2O) n gas-phase processes. Russian Journal of Physical Chemistry A, 2009, 83, 1502-1510.	0.1	1
86	Potential magnetic properties of nanotubes (n, 0) with Klein and Fujita edges. Russian Journal of Physical Chemistry A, 2012, 86, 1261-1267.	0.1	1
87	Study of the geometric structure of the molecules of H2O, Li2O, and LiOH by the method of diatomic fragments in molecules. Journal of Structural Chemistry, 1979, 19, 665-671.	0.3	0
88	Low-temperature properties of wide-cut diesel fuels. Chemistry and Technology of Fuels and Oils, 1983, 19, 429-431.	0.2	0
89	Bonding energy in (Li2OH)ï¿½ complex ions. Journal of Structural Chemistry, 1987, 28, 19-22.	0.3	0
90	Theoretical models of vibrational predissociation for van der Waals complexes. , 1994, , .		0

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91	Modeling the electronic structure of graphite intercalation compounds with lithium by metal complexes with polybenzene systems. Journal of Structural Chemistry, 1996, 37, 392-397.	0.3	0
92	Application of the non-Hermitean effective Hamiltonian method to metastable van der Waals complexes. , 1997, , .		0
93	Structural peculiarities and the possibility of the existence of small water cluster anions (H2O) n â˜' withnâ‰¤4. Russian Chemical Bulletin, 1997, 46, 36-41.	0.4	0
94	The possibility of the existence of (H2O) n â˜' anions withn=5, 6. Russian Chemical Bulletin, 1997, 46, 42-48.	0.4	0
95	Ab-initio-based model for the charge transfer mechanisms in Ar+ + H2O collisions. International Journal of Mass Spectrometry, 2000, 203, 19-29.	0.7	0
96	Title is missing!. Protection of Metals, 2002, 38, 78-82.	0.2	0
97	<title>State of the art in quantum chemistry today</title>. , 2004, 5311, 39.		0
98	Simple molecules on a zeolite acceptor center: A quantum-chemical approach. Russian Journal of Physical Chemistry A, 2007, 81, 1365-1370.	0.1	0
99	The equilibrium structures of the Li[C n]1 (n = 7â€“12) complexes and their alternation depending on n. Russian Journal of Physical Chemistry A, 2009, 83, 77-80.	0.1	0
100	9th International Conference on Fundamental and Applied Aspects of Physical Chemistry: PHYSICAL CHEMISTRY 2008 (Belgrade, September 24â€“26, 2008). Russian Journal of Physical Chemistry A, 2009, 83, 1429-1429.	0.1	0
101	Calculations of predissociative lifetimes of RG...Hal 2 Van der Waals complexes. , 1992, , .		0