

Andrej I Panin

List of Publications by Year in descending order

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185
citing authors

#	ARTICLE	IF	CITATIONS
1	Electronic structure of crystalline uranium nitrides UN, U ₂ N ₃ and U ₂ : LCAO calculations with the basis set optimization. Journal of Physics: Conference Series, 2008, 117, 012015.	0.3	23
2	Electronic structure of crystalline uranium nitride: LCAO DFT calculations. Physica Status Solidi (B): Basic Research, 2008, 245, 114-122.	0.7	22
3	Search for stationary points of arbitrary index by augmented Hessian method. International Journal of Quantum Chemistry, 1995, 54, 329-336.	1.0	21
4	Structures and photophysical properties of 3,4-diaryl-1H-pyrrol-2,5-diimines and 2,3-diarylmaleimides. Journal of Molecular Structure, 2017, 1146, 554-561.	1.8	12
5	A method for calculations of the electronic spectra of transition metal compounds. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1998, 54, 1601-1605.	2.0	10
6	Stability and structures of gaseous In ₂ MoO ₄ , In ₂ WO ₄ and In ₂ W ₂ O ₇ . Dalton Transactions, 2013, 42, 8339.	1.6	10
7	Mass spectrometric study of thermodynamic properties of BaO-CeO ₂ . The formation enthalpy of BaCeO ₃ (solid). Journal of Alloys and Compounds, 2017, 693, 1028-1034.	2.8	10
8	Calculations of electronic structure of the UF ₆ molecule and the UO ₂ crystal with a relativistic pseudopotential. Russian Journal of General Chemistry, 2008, 78, 1823-1835.	0.3	9
9	Thermodynamics of gaseous barium cerate studied by Knudsen effusion mass spectrometry. Rapid Communications in Mass Spectrometry, 2016, 30, 2027-2032.	0.7	9
10	Thermodynamic properties and structure of gaseous BMoO ₄ . Dalton Transactions, 2013, 42, 1210-1214.	1.6	8
11	Gaseous titanium molybdates and tungstates: Thermodynamic properties and structures. Rapid Communications in Mass Spectrometry, 2014, 28, 2636-2644.	0.7	8
12	Thermal stability and structures of gaseous GeB ₂ O ₄ and GeMo ₂ O ₇ . RSC Advances, 2014, 4, 39725-39731.	1.7	7
13	Evaluation of relative electron ionization cross sections for some oxides and oxyacid salts. Rapid Communications in Mass Spectrometry, 2017, 31, 1559-1564.	0.7	7
14	Argentophilic interactions in argentum chalcogenides: First principles calculations and topological analysis of electron density. Journal of Computational Chemistry, 2021, 42, 242-247.	1.5	7
15	Contraction operator over electronic fock space. I. Symmetry properties. International Journal of Quantum Chemistry, 1985, 28, 861-875.	1.0	6
16	Structure of MCSCF electronic energy domain. International Journal of Quantum Chemistry, 1986, 30, 509-541.	1.0	6
17	Thermochemical study of gaseous salts of oxygen-containing acids: XIX. Tin salts. Russian Journal of General Chemistry, 2015, 85, 1351-1369.	0.3	6
18	Thermodynamic properties of the gaseous lead phosphates. Journal of Chemical Thermodynamics, 2016, 101, 337-342.	1.0	6

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19	Method of recurrent construction of L ² wdin spin-adapted wave functions. I. Addition and subtraction operators. <i>International Journal of Quantum Chemistry</i> , 1982, 22, 557-573.	1.0	5
20	Semiempirical version of the multiconfiguration SCF method. <i>Journal of Structural Chemistry</i> , 1990, 31, 1-7.	0.3	5
21	A Quantum-Chemical Study of Dissociation of H ₂ Molecule on Palladium Clusters. <i>Russian Journal of General Chemistry</i> , 2004, 74, 975-979.	0.3	5
22	Rod groups and their settings as special geometric realisations of line groups. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2012, 68, 582-588.	0.3	5
23	Symmetry classification of electron and phonon states in TiO ₂ -based nanowires and nanotubes. <i>Journal of Computational Chemistry</i> , 2015, 36, 957-969.	1.5	5
24	Method of recurrent construction of L ² wdin spin-adapted wave functions. III. L ² wdin basis and its permutation symmetry: Evaluation of overlap integrals. <i>International Journal of Quantum Chemistry</i> , 1983, 24, 279-306.	1.0	4
25	Approximate solution of the representability problem. <i>International Journal of Quantum Chemistry</i> , 2001, 85, 1-17.	1.0	4
26	Thermodynamic study of gaseous tin molybdates by high-temperature mass spectrometry. <i>Rapid Communications in Mass Spectrometry</i> , 2015, 29, 1427-1436.	0.7	4
27	Thermochemical study of gaseous salts of oxygen-containing acids: XXI. Zinc phosphate. <i>Russian Journal of General Chemistry</i> , 2016, 86, 778-784.	0.3	4
28	Thermochemical study of gaseous salts of oxygen-containing acids: XX. Germanium salts. <i>Russian Journal of General Chemistry</i> , 2015, 85, 1588-1598.	0.3	3
29	A nonempirical calculation of the potential surfaces of the exchange reactions of atoms of the elements of the second period with the hydrogen molecule. <i>Journal of Structural Chemistry</i> , 1981, 22, 8-12.	0.3	2
30	Method of recurrent construction of L ² wdin spin-adapted wave functions. II. Local representation of creation-annihilation operators. <i>International Journal of Quantum Chemistry</i> , 1982, 22, 1177-1188.	1.0	2
31	Semiempirical calculations of the electronically excited states of organometallic compounds: Selection of configuration interaction basis sets. <i>Journal of Structural Chemistry</i> , 1996, 37, 181-191.	0.3	2
32	Electronic structure and fluorescence spectrum of the HeO ⁺ cation. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2001, 90, 367-370.	0.2	2
33	Pure representability problem and new models of the electronic Fock space. <i>International Journal of Quantum Chemistry</i> , 2002, 87, 23-36.	1.0	2
34	Effects of electronic correlation on local properties of electronic structure of TiO ₂ and Ti ₂ O ₃ crystals: DFT and post-HF approaches. <i>International Journal of Quantum Chemistry</i> , 2002, 88, 472-480.	1.0	2
35	Electronic Fock spaces: Phase prefactors and new algebraic structure. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 246-259.	1.0	2
36	Electronic Fock space as associative superalgebra. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1786-1794.	1.0	2

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37	Electronic structure of crystalline uranium nitride: LCAO DFT calculations. <i>Journal of Structural Chemistry</i> , 2007, 48, S125-S133.	0.3	2
38	Formation and thermodynamics of gaseous germanium and tin vanadates: a mass spectrometric and quantum chemical study. <i>Dalton Transactions</i> , 2015, 44, 10014-10021.	1.6	2
39	Thermochemical study of gaseous salts of oxygen-containing acids: XXII.1 Lead salts. <i>Russian Journal of General Chemistry</i> , 2016, 86, 2243-2255.	0.3	2
40	Mass spectrometric study of thermodynamic properties of gaseous lead tellurates. Estimation of formation enthalpies of gaseous lead polonates. <i>Journal of Nuclear Materials</i> , 2016, 479, 271-278.	1.3	2
41	Thermodynamic properties of gaseous cerium molybdates and tungstates studied by Knudsen effusion mass spectrometry. <i>Rapid Communications in Mass Spectrometry</i> , 2018, 32, 1608-1616.	0.7	2
42	Thermochemical study of gaseous indium-arsenic sulfosalt. <i>Rapid Communications in Mass Spectrometry</i> , 2019, 33, 1826-1833.	0.7	2
43	Weyl algebra of electronic Fock space: Application to evaluation of matrix elements of spin tensor operators. <i>International Journal of Quantum Chemistry</i> , 1985, 27, 501-525.	1.0	1
44	Contraction operator over electronic Fock space. II. Weak representability problem. <i>International Journal of Quantum Chemistry</i> , 1989, 35, 629-647.	1.0	1
45	Correlation Effects in the Unrestricted Hartree-Fock Method for Solids: Electronic Structure of TiO ₂ Crystal. <i>Physica Status Solidi (B): Basic Research</i> , 1999, 214, r5-r6.	0.7	1
46	1-Density operators and algebraic version of the Hohenberg-Kohn theorem. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 858-874.	1.0	1
47	Quantum chemical modeling of nucleophilic substitution reactions in the complexes cis-Pt(NH ₃) ₂ Cl ₂ and cis-Pd(NH ₃) ₂ Cl ₂ . <i>Russian Chemical Bulletin</i> , 2012, 61, 796-801.	0.4	1
48	Mass spectrometric study of thermodynamic properties of gaseous tin borates SnB ₂ O ₄ and Sn ₂ B ₂ O ₅ . <i>International Journal of Mass Spectrometry</i> , 2015, 392, 69-72.	0.7	1
49	Vapor pressures and thermodynamic properties of simple and complex iodides. <i>Thermochimica Acta</i> , 2021, 703, 178996.	1.2	1
50	Choice of semiempirical parameters for CNDO calculation of the electronic structure of organolithium compounds. <i>Journal of Structural Chemistry</i> , 1977, 18, 243-246.	0.3	0
51	Potential surfaces for the interaction of the atoms of the elements of the first period with the H ₂ molecule (linear arrangement of the atoms). <i>Journal of Structural Chemistry</i> , 1978, 19, 451-454.	0.3	0
52	Method of recurrent construction of Löwdin spin-adapted wave functions. IV. Matrix element evaluation problem. <i>International Journal of Quantum Chemistry</i> , 1984, 25, 767-793.	1.0	0
53	X-OH ₂ ⁺ (X = C, O) cations: Vibrational spectra, stability, and electron capture reactions. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2000, 89, 706-711.	0.2	0
54	New realizations of electronic configuration interaction spaces. <i>International Journal of Quantum Chemistry</i> , 2004, 98, 11-25.	1.0	0

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55	Polynomial approximations of electronic wave functions. Journal of Mathematical Chemistry, 2011, 49, 1599-1623.	0.7	0
56	Thermodynamic properties of gaseous cerium phosphate studied by Knudsen effusion mass spectrometry. Journal of Mass Spectrometry, 2019, 54, 507-519.	0.7	0
57	Thermodynamic properties of gaseous BaSnO ₂ and Ba ₂ O ₂ studied by Knudsen effusion mass spectrometry. Rapid Communications in Mass Spectrometry, 2020, 34, e8716.	0.7	0