Andrei L Tchougreff

List of Publications by Year in Descending Order

103 papers	3,753 citations	17 h-index	60 g-index
122 ext. papers	4,756 ext. citations	2.5 avg, IF	5.79 L-index

#	Paper	IF	Citations
103	Local perturbations of periodic systems. Chemisorption and point defects by GoGreenGo. *Journal of Computational Chemistry*, **2021**, 42, 2352-2368	3.5	
102	Minimum atomic parameter basis sets for elements 1□4 in a Hartree□ock setting. *International Journal of Quantum Chemistry*, **2021**, 121, e26687	2.1	1
101	Solid-state quantum chemistry with □(ThetaPhi): Spin-liquids, superconductors, and magnetic superstructures made computationally available. *Journal of Computational Chemistry*, **2021**, 42, 1498-1513	3.5	1
100	Spatial distribution of atomic electronic density for elements 1□4 as coming from a Hartree□ock treatment within the minimum atomic parameters paradigm. *International Journal of Quantum Chemistry*, **2021**, 121, e26690	2.1	
99	Efficient magnetic superstructure optimization with □*Computational Materials Science*, **2021**, 188, 110140	3.2	2
98	Quantum Metrics for Continuous Shape Measures of Molecules. *Russian Journal of Physical Chemistry A*, **2021**, 95, 1846-1856	0.7	
97	□Solid state package allowing Bardeen□Cooper□chrieffer and magnetic superstructure electronic states. *Computer Physics Communications*, **2020**, 251, 107079	4.2	3
96	Deductive molecular mechanics of carbon allotropes (Review article). *Low Temperature Physics*, **2020**, 46, 655-670	0.7	2
95	Magnetic Properties of Quasi-One-Dimensional Crystals Formed by Graphene Nanoclusters and Embedded Atoms of the Transition Metals. *Crystals*, **2019**, 9, 251	2.3	4
94	Relative stability of diamond and graphite as seen through bonds and hybridizations. *Physical Chemistry Chemical Physics*, **2019**, 21, 10961-10969	3.6	8
93	Deductive molecular mechanics of four-coordinated carbon allotropes. *Physical Chemistry Chemical Physics*, **2019**, 21, 18138-18148	3.6	3
92	cartesius fort - object fortran Library for Chemistry and Materials Science. *Lecture Notes in Computer Science*, **2019**, 639-651	0.9	2
91	The gapless energy spectrum and spin-Peierls instability of 1D Heisenberg spin systems in polymeric complexes of transition metals and hypothetical carbon allotropes. *Journal of Physics Condensed Matter*, **2019**, 31, 305601	1.8	6
90	Atomic orbitals revisited: generalized hydrogen-like basis sets for 2nd-row elements. *Theoretical Chemistry Accounts*, **2019**, 138, 1	1.9	6
89	De glaci□us or deductive molecular mechanics of ice polymorphs. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	1
88	Magnetic inhomogeneity in the copper pseudochalcogenide CuNCN. *Physical Review B*, **2018**, 97,	3.3	4
87	Applying group functions to description of ionic liquids. *Computational and Theoretical Chemistry*, **2017**, 1116, 141-150	2	3

86	Atomic motions in the layered copper pseudochalcogenide CuNCN indicative of a quantum spin-liquid scenario. *Journal of Physics Condensed Matter*, **2017**, 29, 235701	1.8	5
85	Instrumental resolution as a function of scattering angle and wavelength as exemplified for the POWGEN instrument. *Journal of Applied Crystallography*, **2017**, 50, 866-875	3.8	4
84	Resonating Valence Bonds in Chemistry and Solid State **2017**, 87-117		
83	[illegible]or deductive molecular mechanics of crystalline water **2017**,		2
82	Two theorems about C2 and some more. *Molecular Physics*, **2016**, 114, 1423-1444	1.7	9
81	Several stories from theoretical chemistry with some Russian flavor and implications for theorems of chemistry, vagueness of its concepts, fuzziness of its definitions, iconicity of its language, and peculiarities of its nomenclature. *International Journal of Quantum Chemistry*, **2016**, 116, 137-160	2.1	8
80	Effective hamiltonian crystal field: Present status and applications to iron compounds. *International Journal of Quantum Chemistry*, **2016**, 116, 282-294	2.1	6
79	Benchmarks of graph invariants for hydrogen-bond networks in water clusters of different topology. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	2
78	A Rietveld refinement method for angular- and wavelength-dispersive neutron time-of-flight powder diffraction data. *Journal of Applied Crystallography*, **2015**, 48, 1627-1636	3.8	8
77	Magnetism and lattice dynamics of FeNCN compared to FeO. *New Journal of Chemistry*, **2014**, 38, 4670-4677	3.0	10
76	Magneto-optical response of 3d-decorated polyoxomolybdates with [illegible]Keggin structure. *Inorganic Chemistry*, **2014**, 53, 2892-8	5.1	1
75	Effective Hamiltonian crystal fields: Present status and applicability to magnetic interactions in polynuclear transition metal complexes. *Russian Journal of Physical Chemistry A*, **2014**, 88, 1904-1913	0.7	4
74	Mean-field RVB ground states of lattice models of CuNCN. *Low Temperature Physics*, **2014**, 40, 73-83	0.7	4
73	Effective Hamiltonian Crystal Field as applied to magnetic exchange parameters in [illegible]oxo-bridged Cr(III) dimers. *Journal of Physical Chemistry A*, **2013**, 117, 7980-8	2.8	10
72	Analytic projection from plane-wave and PAW wavefunctions and application to chemical-bonding analysis in solids. *Journal of Computational Chemistry*, **2013**, 34, 2557-67	3.5	790
71	Resonance theory of catalytic action of transition-metal complexes: Isomerization of quadricyclane to norbornadiene catalyzed by metal porphyrins. *International Journal of Quantum Chemistry*, **2013**, 113, 1833-1846	2.1	7
70	Low-temperature structure anomalies in CuNCN. Manifestations of RVB phase transitions?. *Journal of Physics Condensed Matter*, **2013**, 25, 435602	1.8	5
69	High-resolution neutron diffraction study of CuNCN: new evidence of structure anomalies at low temperature. *Journal of Chemical Physics*, **2013**, 139, 224707	3.9	9

68	Structural Study of CuNCN and Its Theoretical Implications: A Case of a Resonating-Valence-Bond State?. *Journal of Physical Chemistry Letters*, **2012**, 3, 3360-3366	6.4	10
67	Syntheses, Crystal Structures and Magnetic Properties of Cr(NCNH2)4Cl2 and Mn(NCNH2)4Cl2. *Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences*, **2012**, 67, 1205-1211	1	2
66	Phenomenological model of spin crossover in molecular crystals as derived from atom-atom potentials. *Physical Chemistry Chemical Physics*, **2011**, 13, 13238-46	3.6	7
65	Crystal orbital Hamilton population (COHP) analysis as projected from plane-wave basis sets. *Journal of Physical Chemistry A*, **2011**, 115, 5461-6	2.8	1057
64	Crystal and electronic structure of the room temperature organometallic ferrimagnet V(TCNE)2. Analysis of numerical DoS and magnetic properties as related to orbital and spin-Hamiltonian models. *International Journal of Quantum Chemistry*, **2011**, 111, 2490-2509	2.1	1
63	d-d Spectra of transition-metal carbodiimides and hydrocyanamides as derived from many-particle effective Hamiltonian calculations. *Journal of Physical Chemistry A*, **2011**, 115, 4547-52	2.8	6
62	Unconventional magnetism in a nitrogen-containing analog of cupric oxide. *Physical Review Letters*, **2011**, 107, 047208	7.4	19
61	Synthesis, characterization, and quantum-chemical studies of Ni(CN)2MX (M = Rb, Cs; X = Cl, Br). *Inorganic Chemistry*, **2010**, 49, 7414-23	5.1	0
60	Electronic and magnetic structure of transition-metal carbodiimides by means of GGA+U theory. *Journal of Physical Chemistry A*, **2010**, 114, 12345-52	2.8	15
59	Hydrogen-bond networks in water clusters (H2O)20: an exhaustive quantum-chemical analysis. *ChemPhysChem*, **2010**, 11, 384-8	3.2	42
58	Experimental and Quantum-Chemical Investigations of the UV/Vis Absorption Spectrum of Manganese Carbodiimide, MnNCN *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2010**, 636, 343-348	1.2	21
57	Classes of admissible exchange-correlation density functionals for pure spin and angular momentum states. *International Journal of Quantum Chemistry*, **2010**, 110, 454-475	2.1	5
56	Nephelauxetic effect revisited. *International Journal of Quantum Chemistry*, **2009**, 109, 2606-2621	2.1	33
55	Multipole model for the electron group functions method. *Journal of Physical Chemistry A*, **2009**, 113, 11406-15	2.8	9
54	Modeling molecular crystals formed by spin-active metal complexes by atom-atom potentials. *Physical Chemistry Chemical Physics*, **2009**, 11, 10983-93	3.6	7
53	Hybrid Methods of Molecular Modeling. *Progress in Theoretical Chemistry and Physics*, **2008**,	0.6	19
52	A computational study of the crystal and electronic structure of the room temperature organometallic ferromagnet V(TCNE)2. *Journal of Computational Chemistry*, **2008**, 29, 2220-33	3.5	12
51	Deriving a mechanistic model for potential energy surface of coordination compounds of nontransition elements. *International Journal of Quantum Chemistry*, **2007**, 107, 2519-2538	2.1	3

50	Towards a possible ab initio molecular mechanics. Transferability of density matrix elements. *International Journal of Quantum Chemistry*, **2007**, 107, 2539-2555	2.1	5
49	New generation of semiempirical methods of molecular modeling based on the theory of group functions. *Journal of Structural Chemistry*, **2007**, 48, S32-S54	0.9	8
48	Group functions approach based on the combination of strictly local geminals and molecular orbitals. *International Journal of Quantum Chemistry*, **2006**, 106, 571-587	2.1	13
47	MNDO parameterized hybrid SLG/SCF method as used for molecular modeling of Zn(II) complexes. *International Journal of Quantum Chemistry*, **2006**, 106, 2268-2280	2.1	2
46	Efficient multipole model and linear scaling of NDDO-based methods. *Journal of Physical Chemistry A*, **2005**, 109, 7613-20	2.8	15
45	Transferability of parameters of strictly local geminals in wave function and possibility of sequential derivation of molecular mechanics. *Journal of Computational Chemistry*, **2005**, 26, 491-505	3.5	9
44	Transition metal complexes with open d-shell in semiempirical context. Application to analysis of Mössbauer data on spin-active iron(II) compounds. *Theoretical Chemistry Accounts*, **2005**, 114, 97-109	1.9	6
43	Deductive molecular mechanics of sp3 carbon atom. *International Journal of Quantum Chemistry*, **2004**, 96, 175-184	2.1	11
42	Deductive molecular mechanics of sp3 nitrogen atom and its application to analysis of a QM/MM interface. *International Journal of Quantum Chemistry*, **2004**, 100, 667-676	2.1	4
41	Local Effective Crystal Field Combined with Molecular Mechanics. Improved QM/MM Junction and Application to Fe(II) and Co(II) Complexes. *Journal of Physical Chemistry A*, **2004**, 108, 6351-6364	2.8	16
40	Low- and high-spin iron (II) complexes studied by effective crystal field method combined with molecular mechanics. *Journal of Computational Chemistry*, **2003**, 24, 1703-19	3.5	9
39	Local many-electron states in transition metal oxides and their surface complexes with atomic and molecular oxygen. *Journal of Solid State Chemistry*, **2003**, 176, 633-645	3.3	8
38	SO(4) group and deductive molecular mechanics. *Computational and Theoretical Chemistry*, **2003**, 630, 243-263		14
37	Deductive molecular mechanics as applied to develop QM/MM picture of dative and coordination bonds. *Computational and Theoretical Chemistry*, **2003**, 632, 91-109		5
36	Fast NDDO Method for Molecular Structure Calculations Based on Strictly Localized Geminals. *Journal of Physical Chemistry A*, **2003**, 107, 358-365	2.8	25
35	Physical Principles of Constructing Hybrid QM/MM Procedures. *Progress in Theoretical Chemistry and Physics*, **2003**, 207-245	0.6	3
34	Effective crystal field for trivalent first transition row ions. *International Journal of Quantum Chemistry*, **2002**, 88, 370-379	2.1	8
33	Generic molecular mechanics as based on local quantum description of molecular electronic structure. *International Journal of Quantum Chemistry*, **2002**, 88, 403-413	2.1	13

32	Hybrid molecular mechanics: For effective crystal field method for modeling potential energy surfaces of transition metal complexes. *International Journal of Quantum Chemistry*, **2002**, 88, 588-605	2.1	10
31	Physical Principles of Constructing Hybrid QM/MM Methods. *Journal of Computational Methods in Sciences and Engineering*, **2002**, 2, 309-314	0.3	
30	Ionization potentials within semiempirical antisymmetrized product of strictly localized geminals approach. *International Journal of Quantum Chemistry*, **2001**, 85, 109-117	2.1	8
29	Potential energy surfaces in hybrid quantum mechanical/molecular mechanical methods. *International Journal of Quantum Chemistry*, **2001**, 84, 39-47	2.1	12
28	Effective Hamiltonian approach to catalytic activity of transition metal complexes. *International Journal of Quantum Chemistry*, **2001**, 84, 99-109	2.1	5
27	Semiempirical implementation of strictly localized geminals for analysis of molecular electronic structure. *Journal of Computational Chemistry*, **2001**, 22, 752-764	3.5	28
26	Effective electronic Hamiltonian for quantum subsystem in hybrid QM/MM methods as derived from APSLG description of electronic structure of classical part of molecular system. *Computational and Theoretical Chemistry*, **2000**, 506, 17-34		12
25	Group functions, L□wdin partition, and hybrid QC/MM methods for large molecular systems. *Physical Chemistry Chemical Physics*, **1999**, 1, 1051-1060	3.6	23
24	d-d spectra of transition metal oxides by effective crystal field method. *Journal of Molecular Catalysis A*, **1997**, 119, 377-386		8
23	The Effective Crystal Field Methodology as Used to Incorporate Transition Metals Into Molecular Mechanics **1997**, 217-232		3
22	Charge Density Wave State of Monolayers in Graphite Intercalation Compounds. *The Journal of Physical Chemistry*, **1996**, 100, 14048-14055		7
21	Quantum mechanical models in catalysis. *Russian Chemical Bulletin*, **1996**, 45, 505-510	1.7	
20	Quantum mechanical models in catalysis. *International Journal of Quantum Chemistry*, **1996**, 57, 413-422	2.1	4
19	Crystal-field splittings and optical spectra of transition-metal mixed-ligand complexes by effective Hamiltonian method. *International Journal of Quantum Chemistry*, **1996**, 57, 663-671	2.1	19
18	Lattice relaxation and order in the low-spin to high-spin transitions in molecular crystals. *International Journal of Quantum Chemistry*, **1996**, 57, 903-912	2.1	7
17	Quantum mechanical models for organometallic reactivity. *International Journal of Quantum Chemistry*, **1996**, 58, 67-84	2.1	7
16	Ground-state multiplicities and d□ excitations of transition-metal complexes by effective Hamiltonian method. *International Journal of Quantum Chemistry*, **1996**, 58, 161-173	2.1	23
15	High-spin-low-spin transitions in Fe(II) complexes by effective Hamiltonian method. *Chemical Physics*, **1995**, 193, 19-26	2.3	21

14	Conductivity in quasi-one-dimensional organic metals. A new approach. *Journal of Chemical Physics*, **1994**, 100, 2223-2231	3.9	
13	Toward a theory of the room-temperature organometallic charge-transfer ferromagnet. *The Journal of Physical Chemistry*, **1993**, 97, 350-356		16
12	The origin of cooperativity in high-spin low-spin transitions in molecular crystals. *Chemical Physics Letters*, **1993**, 214, 627-630	2.5	9
11	A model for CO insertion in transition metal complexes. *Journal of Organometallic Chemistry*, **1993**, 455, 261-270	2.3	8
10	Intra-atomic exchange and ferromagnetic interaction in metallocene-based donor-acceptor stacked crystals. *Physical Review B*, **1992**, 46, 5357-5365	3.3	17
9	Heisenberg Hamiltonian for charge-transfer organometallic ferromagnets. *Journal of Chemical Physics*, **1992**, 96, 6026-6032	3.9	13
8	Charge and spin density waves in the electronic structure of graphite: application to analysis of STM images. *The Journal of Physical Chemistry*, **1992**, 96, 8993-8998		49
7	Electronic structure and optical spectra of transition metal complexes by the effective Hamiltonian method. *Theoretica Chimica Acta*, **1992**, 83, 389-416		45
6	Paramagnetic contribution to the magnetic susceptibility of Bechgaard salts. *Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics*, **1992**, 14, 833-842		2
5	Ferromagnetism of charge-transfer crystals. *Chemical Physics*, **1991**, 153, 371-378	2.3	4
4	On the different types of states of a one dimensional system of electrons in the Hartree-Fock method. *Theoretical and Experimental Chemistry*, **1990**, 25, 475-481	1.3	2
3	Theoretical analysis of catalytic activity of transition metal complexes in symmetry forbidden reactions. *Chemical Physics*, **1989**, 133, 77-87	2.3	7
2	Electronic structure of karbin in the unrestricted Hartree-Fock approximation. *Journal of Structural Chemistry*, **1989**, 30, 377-380	0.9	2
1	or deductive molecular mechanics of crystalline water		1