Andrei L Tchougreff

List of Publications by Citations

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	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
102	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
101	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
100	Electronic structure and optical spectra of transition metal complexes by the effective Hamiltonian method. *Theoretica Chimica Acta*, **1992**, 83, 389-416		45
99	Hydrogen-bond networks in water clusters (H2O)20: an exhaustive quantum-chemical analysis. *ChemPhysChem*, **2010**, 11, 384-8	3.2	42
98	Nephelauxetic effect revisited. *International Journal of Quantum Chemistry*, **2009**, 109, 2606-2621	2.1	33
97	Semiempirical implementation of strictly localized geminals for analysis of molecular electronic structure. *Journal of Computational Chemistry*, **2001**, 22, 752-764	3.5	28
96	Fast NDDO Method for Molecular Structure Calculations Based on Strictly Localized Geminals. *Journal of Physical Chemistry A*, **2003**, 107, 358-365	2.8	25
95	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
94	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
93	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	1.3	21
92	High-spin-low-spin transitions in Fe(II) complexes by effective Hamiltonian method. *Chemical Physics*, **1995**, 193, 19-26	2.3	21
91	Unconventional magnetism in a nitrogen-containing analog of cupric oxide. *Physical Review Letters*, **2011**, 107, 047208	7.4	19
90	Hybrid Methods of Molecular Modeling. *Progress in Theoretical Chemistry and Physics*, **2008**,	0.6	19
89	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
88	Intra-atomic exchange and ferromagnetic interaction in metallocene-based donor-acceptor stacked crystals. *Physical Review B*, **1992**, 46, 5357-5365	3.3	17
87	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

86	Toward a theory of the room-temperature organometallic charge-transfer ferromagnet. *The Journal of Physical Chemistry*, **1993**, 97, 350-356		16
85	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
84	Efficient multipole model and linear scaling of NDDO-based methods. *Journal of Physical Chemistry A*, **2005**, 109, 7613-20	2.8	15
83	SO(4) group and deductive molecular mechanics. *Computational and Theoretical Chemistry*, **2003**, 630, 243-263		14
82	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
81	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
80	Heisenberg Hamiltonian for charge-transfer organometallic ferromagnets. *Journal of Chemical Physics*, **1992**, 96, 6026-6032	3.9	13
79	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
78	Potential energy surfaces in hybrid quantum mechanical/molecular mechanical methods. *International Journal of Quantum Chemistry*, **2001**, 84, 39-47	2.1	12
77	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
76	Deductive molecular mechanics of sp3 carbon atom. *International Journal of Quantum Chemistry*, **2004**, 96, 175-184	2.1	11
75	Magnetism and lattice dynamics of FeNCN compared to FeO. *New Journal of Chemistry*, **2014**, 38, 4670-4677	3.3	10
74	Effective Hamiltonian Crystal Field as applied to magnetic exchange parameters in μ-oxo-bridged Cr(III) dimers. *Journal of Physical Chemistry A*, **2013**, 117, 7980-8	2.8	10
73	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
72	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
71	Two theorems about C2 and some more. *Molecular Physics*, **2016**, 114, 1423-1444	1.7	9
70	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
69	Multipole model for the electron group functions method. *Journal of Physical Chemistry A*, **2009**, 113, 11406-15	2.8	9

68	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
67	Transferability of parameters of strictly local geminals wave function and possibility of sequential derivation of molecular mechanics. *Journal of Computational Chemistry*, **2005**, 26, 491-505	3.5	9
66	The origin of cooperativity in high-spin low-spin transitions in molecular crystals. *Chemical Physics Letters*, **1993**, 214, 627-630	2.5	9
65	Relative stability of diamond and graphite as seen through bonds and hybridizations. *Physical Chemistry Chemical Physics*, **2019**, 21, 10961-10969	3.6	8
64	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
63	d-d spectra of transition metal oxides by effective crystal field method. *Journal of Molecular Catalysis A*, **1997**, 119, 377-386		8
62	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
61	Effective crystal field for trivalent first transition row ions. *International Journal of Quantum Chemistry*, **2002**, 88, 370-379	2.1	8
60	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
59	Ionization potentials within semiempirical antisymmetrized product of strictly localized geminals approach. *International Journal of Quantum Chemistry*, **2001**, 85, 109-117	2.1	8
58	A model for CO insertion in transition metal complexes. *Journal of Organometallic Chemistry*, **1993**, 455, 261-270	2.3	8
57	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
56	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
55	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
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	Charge Density Wave State of Monolayers in Graphite Intercalation Compounds. *The Journal of Physical Chemistry*, **1996**, 100, 14048-14055		7
52	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
51	Quantum mechanical models for organometallic reactivity. *International Journal of Quantum Chemistry*, **1996**, 58, 67-84	2.1	7

50	Theoretical analysis of catalytic activity of transition metal complexes in symmetry forbidden reactions. *Chemical Physics*, **1989**, 133, 77-87	2.3	7
49	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
48	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
47	Transition metal complexes with open d-shell in semiempirical context. Application to analysis of Mössbauer data on spin□ctive iron(II) compounds. *Theoretical Chemistry Accounts*, **2005**, 114, 97-109	1.9	6
46	Effective hamiltonian crystal field: Present status and applications to iron compounds. *International Journal of Quantum Chemistry*, **2016**, 116, 282-294	2.1	6
45	Atomic orbitals revisited: generalized hydrogen-like basis sets for 2nd-row elements. *Theoretical Chemistry Accounts*, **2019**, 138, 1	1.9	6
44	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
43	Low-temperature structure anomalies in CuNCN. Manifestations of RVB phase transitions?. *Journal of Physics Condensed Matter*, **2013**, 25, 435602	1.8	5
42	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
41	Towards a possible ab initio molecular mechanics. Transferability of density matrix elements. *International Journal of Quantum Chemistry*, **2007**, 107, 2539-2555	2.1	5
40	Deductive molecular mechanics as applied to develop QM/MM picture of dative and coordination bonds. *Computational and Theoretical Chemistry*, **2003**, 632, 91-109		5
39	Effective Hamiltonian approach to catalytic activity of transition metal complexes. *International Journal of Quantum Chemistry*, **2001**, 84, 99-109	2.1	5
38	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
37	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
36	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
35	Mean-field RVB ground states of lattice models of CuNCN. *Low Temperature Physics*, **2014**, 40, 73-83	0.7	4
34	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
33	Quantum mechanical models in catalysis. *International Journal of Quantum Chemistry*, **1996**, 57, 413-422	2.1	4

32	Ferromagnetism of charge-transfer crystals. *Chemical Physics*, **1991**, 153, 371-378	2.3	4
31	Magnetic inhomogeneity in the copper pseudochalcogenide CuNCN. *Physical Review B*, **2018**, 97,	3.3	4
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29	Deductive molecular mechanics of four-coordinated carbon allotropes. *Physical Chemistry Chemical Physics*, **2019**, 21, 18138-18148	3.6	3
28	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
27	The Effective Crystal Field Methodology as Used to Incorporate Transition Metals Into Molecular Mechanics **1997**, 217-232		3
26	Physical Principles of Constructing Hybrid QM/MM Procedures. *Progress in Theoretical Chemistry and Physics*, **2003**, 207-245	0.6	3
25	Solid state package allowing BardeenCooperSchrieffer and magnetic superstructure electronic states. *Computer Physics Communications*, **2020**, 251, 107079	4.2	3
24	Benchmarks of graph invariants for hydrogen-bond networks in water clusters of different topology. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	2
23	cartesius fort - object fortran Library for Chemistry and Materials Science. *Lecture Notes in Computer Science*, **2019**, 639-651	0.9	2
22	or deductive molecular mechanics of crystalline water **2017**,		2
21	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
20	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
19	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
18	Electronic structure of karbin in the unrestricted Hartree-Fock approximation. *Journal of Structural Chemistry*, **1989**, 30, 377-380	0.9	2
17	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
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15	Efficient magnetic superstructure optimization with *Computational Materials Science*, **2021**, 188, 110140	3.2	2

14	Magneto-optical response of 3d-decorated polyoxomolybdates with Keggin structure. *Inorganic Chemistry*, **2014**, 53, 2892-8	5.1	1
13	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
12	[illegible]or deductive molecular mechanics of crystalline water		1
11	Minimum atomic parameter basis sets for elements 1–54 in a Hartree–Fock setting. *International Journal of Quantum Chemistry*, **2021**, 121, e26687	2.1	1
10	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
9	De glaciBus or deductive molecular mechanics of ice polymorphs. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	1
8	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
7	Resonating Valence Bonds in Chemistry and Solid State **2017**, 87-117		
6	Physical Principles of Constructing Hybrid QM/MM Methods. *Journal of Computational Methods in Sciences and Engineering*, **2002**, 2, 309-314	0.3	
5	Quantum mechanical models in catalysis. *Russian Chemical Bulletin*, **1996**, 45, 505-510	1.7	
4	Conductivity in quasi-one-dimensional organic metals. A new approach. *Journal of Chemical Physics*, **1994**, 100, 2223-2231	3.9	
3	Local perturbations of periodic systems. Chemisorption and point defects by GoGreenGo. *Journal of Computational Chemistry*, **2021**, 42, 2352-2368	3.5	
2	Spatial distribution of atomic electronic density for elements 1–54 as coming from a Hartree–Fock treatment within the minimum atomic parameters paradigm. *International Journal of Quantum Chemistry*, **2021**, 121, e26690	2.1	
1	Quantum Metrics for Continuous Shape Measures of Molecules. *Russian Journal of Physical Chemistry A*, **2021**, 95, 1846-1856	0.7	