Andrei L TchougrÃ©eff

List of Publications by Year
in descending order

105 papers	5,886 citations	430442 18 h-index	76769 74 g-index
122 all docs	122 docs citations	122 times ranked	4264 citing authors

#	Article	IF	Citations
1	Crystal Orbital Hamilton Population (COHP) Analysis As Projected from Plane-Wave Basis Sets. Journal of Physical Chemistry A, 2011, 115, 5461-5466.	1.1	1,823
2	LOBSTER: A tool to extract chemical bonding from planeâ€wave based DFT. Journal of Computational Chemistry, 2016, 37, 1030-1035.	1.5	1,791
3	Analytic projection from plane-wave and PAW wavefunctions and application to chemical-bonding analysis in solids. Journal of Computational Chemistry, 2013, 34, 2557-2567.	1.5	1,178
4	Electronic structure and optical spectra of transition metal complexes by the effective Hamiltonian method. Theoretica Chimica Acta, 1992, 83, 389-416.	0.9	54
5	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.	2.9	53
6	Hydrogenâ€Bond Networks in Water Clusters (H₂O)₂₀: An Exhaustive Quantumâ€Chemical Analysis. ChemPhysChem, 2010, 11, 384-388.	1.0	50
7	Nephelauxetic effect revisited. International Journal of Quantum Chemistry, 2009, 109, 2606-2621.	1.0	36
8	Semiempirical implementation of strictly localized geminals for analysis of molecular electronic structure. Journal of Computational Chemistry, 2001, 22, 752-764.	1.5	31
9	Fast NDDO Method for Molecular Structure Calculations Based on Strictly Localized Geminals. Journal of Physical Chemistry A, 2003, 107, 358-365.	1.1	27
10	Ground-state multiplicities andd?d excitations of transition-metal complexes by effective Hamiltonian method. International Journal of Quantum Chemistry, 1996, 58, 161-173.	1.0	26
11	Group functions, LÃ¶wdin partition, and hybrid QC/MM methods for large molecular systems. Physical Chemistry Chemical Physics, 1999, 1, 1051-1060.	1.3	26
12	High-spin-low-spin transitions in Fe(II) complexes by effective Hamiltonian method. Chemical Physics, 1995, 193, 19-26.	0.9	25
13	Experimental and Quantumâ€Chemical Investigations of the UV/Vis Absorption Spectrum of Manganese Carbodiimide, MnNCNÂ. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2010, 636, 343-348.	0.6	23
14	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.	1.0	22
15	Unconventional Magnetism in a Nitrogen-Containing Analog of Cupric Oxide. Physical Review Letters, 2011, 107, 047208.	2.9	22
16	Intra-atomic exchange and ferromagnetic interaction in metallocene-based donor-acceptor stacked crystals. Physical Review B, 1992, 46, 5357-5365.	1.1	21
17	Electronic and Magnetic Structure of Transition-Metal Carbodiimides by Means of GGA+U Theory. Journal of Physical Chemistry A, 2010, 114, 12345-12352.	1.1	21
18	Relative stability of diamond and graphite as seen through bonds and hybridizations. Physical Chemistry Chemical Physics, 2019, 21, 10961-10969.	1.3	20

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19	Heisenberg Hamiltonian for chargeâ€transfer organometallic ferromagnets. Journal of Chemical Physics, 1992, 96, 6026-6032.	1.2	18
20	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.	1.1	18
21	Toward a theory of the room-temperature organometallic charge-transfer ferromagnet. The Journal of Physical Chemistry, 1993, 97, 350-356.	2.9	17
22	SO(4) group and deductive molecular mechanics. Computational and Theoretical Chemistry, 2003, 630, 243-263.	1.5	17
23	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.	1.5	16
24	Efficient Multipole Model and Linear Scaling of NDDO-Based Methods. Journal of Physical Chemistry A, 2005, 109, 7613-7620.	1.1	16
25	Deductive molecular mechanics of sp3carbon atom. International Journal of Quantum Chemistry, 2004, 96, 175-184.	1.0	15
26	Generic molecular mechanics as based on local quantum description of molecular electronic structure. International Journal of Quantum Chemistry, 2002, 88, 403-413.	1.0	14
27	Group functions approach based on the combination of strictly local geminals and molecular orbitals. International Journal of Quantum Chemistry, 2006, 106, 571-587.	1.0	14
28	Magnetism and lattice dynamics of FeNCN compared to FeO. New Journal of Chemistry, 2014, 38, 4670-4677.	1.4	14
29	Potential energy surfaces in hybrid quantum mechanical/molecular mechanical methods. International Journal of Quantum Chemistry, 2001, 84, 39-47.	1.0	13
30	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.	1.0	12
31	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.	1.5	12
32	A computational study of the crystal and electronic structure of the room temperature organometallic ferromagnet V(TCNE)₂. Journal of Computational Chemistry, 2008, 29, 2220-2233.	1.5	12
33	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.	2.1	12
34	Effective Hamiltonian Crystal Field As Applied to Magnetic Exchange Parameters in Î¼-Oxo-Bridged Cr(III) Dimers. Journal of Physical Chemistry A, 2013, 117, 7980-7988.	1.1	12
35	Low- and high-spin iron (II) complexes studied by effective crystal field method combined with molecular mechanics. Journal of Computational Chemistry, 2003, 24, 1703-1719.	1.5	11
36	High-resolution neutron diffraction study of CuNCN: New evidence of structure anomalies at low temperature. Journal of Chemical Physics, 2013, 139, 224707.	1.2	11

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37	Two theorems about C₂ and some more. Molecular Physics, 2016, 114, 1423-1444.	0.8	11
38	Theoretical analysis of catalytic activity of transition metal complexes in symmetry forbidden reactions. Chemical Physics, 1989, 133, 77-87.	0.9	10
39	Quantum mechanical models for organometallic reactivity. International Journal of Quantum Chemistry, 1996, 58, 67-84.	1.0	10
40	d-d spectra of transition metal oxides by effective crystal field method. Journal of Molecular Catalysis A, 1997, 119, 377-386.	4.8	10
41	Effective crystal field for trivalent first transition row ions. International Journal of Quantum Chemistry, 2002, 88, 370-379.	1.0	10
42	New generation of semiempirical methods of molecular modeling based on the theory of group functions. Journal of Structural Chemistry, 2007, 48, S32-S54.	0.3	10
43	Multipole Model for the Electron Group Functions Method. Journal of Physical Chemistry A, 2009, 113, 11406-11415.	1.1	10
44	A Rietveld refinement method for angular- and wavelength-dispersive neutron time-of-flight powder diffraction data. Journal of Applied Crystallography, 2015, 48, 1627-1636.	1.9	10
45	Effective hamiltonian crystal field: Present status and applications to iron compounds. International Journal of Quantum Chemistry, 2016, 116, 282-294.	1.0	10
46	The origin of cooperativity in high-spinâ€"low-spin transitions in molecular crystals. Chemical Physics Letters, 1993, 214, 627-630.	1.2	9
47	A model for CO insertion in transition metal complexes. Journal of Organometallic Chemistry, 1993, 455, 261-270.	0.8	9
48	Ionization potentials within semiempirical antisymmetrized product of strictly localized geminals approach. International Journal of Quantum Chemistry, 2001, 85, 109-117.	1.0	9
49	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.	1.4	9
50	dâ^'d Spectra of Transition-Metal Carbodiimides and Hydrocyanamides as Derived from Many-Particle Effective Hamiltonian Calculations. Journal of Physical Chemistry A, 2011, 115, 4547-4552.	1.1	9
51	Resonance theory of catalytic action of transitionâ€"metal complexes: Isomerization of quadricyclane to norbornadiene catalyzed by metal porphyrins. International Journal of Quantum Chemistry, 2013, 113, 1833-1846.	1.0	9
52	Several stories from theoretical chemistry with some <scp>R</scp>ussian 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.	1.0	9
53	Magnetic Properties of Quasi-One-Dimensional Crystals Formed by Graphene Nanoclusters and Embedded Atoms of the Transition Metals. Crystals, 2019, 9, 251.	1.0	9
54	Charge Density Wave State of Monolayers in Graphite Intercalation Compounds. The Journal of Physical Chemistry, 1996, 100, 14048-14055.	2.9	8

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55	Deductive molecular mechanics as applied to develop QM/MM picture of dative and coordination bonds. Computational and Theoretical Chemistry, 2003, 632, 91-109.	1.5	8
56	Transition metal complexes with open d-shell in semiempirical context. Application to analysis of MÃ¶ssbauer data on spinâ€“active iron(II) compounds. Theoretical Chemistry Accounts, 2005, 114, 97-109.	0.5	8
57	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.	0.7	8
58	Atomic orbitals revisited: generalized hydrogen-like basis sets for 2nd-row elements. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	8
59	Lattice relaxation and order in the low-spin to high-spin transitions in molecular crystals. International Journal of Quantum Chemistry, 1996, 57, 903-912.	1.0	7
60	Deductive molecular mechanics of sp3nitrogen atom and its application to analysis of a QM/MM interface. International Journal of Quantum Chemistry, 2004, 100, 667-676.	1.0	7
61	Modeling molecular crystals formed by spin-active metal complexes by atomâ€“atom potentials. Physical Chemistry Chemical Physics, 2009, 11, 10983.	1.3	7
62	Phenomenological model of spin crossover in molecular crystals as derived from atomâ€“atom potentials. Physical Chemistry Chemical Physics, 2011, 13, 13238.	1.3	7
63	Instrumental resolution as a function of scattering angle and wavelength as exemplified for the POWGEN instrument. Journal of Applied Crystallography, 2017, 50, 866-875.	1.9	6
64	Physical Principles of Constructing Hybrid QM/MM Procedures. Progress in Theoretical Chemistry and Physics, 2003, , 207-245.	0.2	6
65	Ferromagnetism of charge-transfer crystals. Chemical Physics, 1991, 153, 371-378.	0.9	5
66	Quantum mechanical models in catalysis. International Journal of Quantum Chemistry, 1996, 57, 413-422.	1.0	5
67	Effective Hamiltonian approach to catalytic activity of transition metal complexes. International Journal of Quantum Chemistry, 2001, 84, 99-109.	1.0	5
68	Deriving a mechanistic model for potential energy surface of coordination compounds of nontransition elements. International Journal of Quantum Chemistry, 2007, 107, 2519-2538.	1.0	5
69	Towards a possibleab initio molecular mechanics. Transferability of density matrix elements. International Journal of Quantum Chemistry, 2007, 107, 2539-2555.	1.0	5
70	Classes of admissible exchangeâ€correlation density functionals for pure spin and angular momentum states. International Journal of Quantum Chemistry, 2010, 110, 454-475.	1.0	5
71	Low-temperature structure anomalies in CuNCN. Manifestations of RVB phase transitions?. Journal of Physics Condensed Matter, 2013, 25, 435602.	0.7	5
72	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.	0.1	5

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73	Atomic motions in the layered copper pseudochalcogenide CuNCN indicative of a quantum spin-liquid scenario. Journal of Physics Condensed Matter, 2017, 29, 235701.	0.7	5
74	Mean-field RVB ground states of lattice models of CuNCN. Low Temperature Physics, 2014, 40, 73-83.	0.2	4
75	Benchmarks of graph invariants for hydrogen-bond networks in water clusters of different topology. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	4
76	Magnetic inhomogeneity in the copper pseudochalcogenide CuNCN. Physical Review B, 2018, 97, .	1.1	4
77	Deductive molecular mechanics of four-coordinated carbon allotropes. Physical Chemistry Chemical Physics, 2019, 21, 18138-18148.	1.3	4
78	ÎĴ¦: Solid state package allowing Bardeenâ€“Cooperâ€“Schrieffer and magnetic superstructure electronic states. Computer Physics Communications, 2020, 251, 107079.	3.0	4
79	MNDO parameterized hybrid SLG/SCF method as used for molecular modeling of Zn(II) complexes. International Journal of Quantum Chemistry, 2006, 106, 2268-2280.	1.0	3
80	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.	0.3	3
81	Applying group functions to description of ionic liquids. Computational and Theoretical Chemistry, 2017, 1116, 141-150.	1.1	3
82	ÎĴµÏĴ¯ Ï„Î¿Ï… ÏƒÏ„Î¿Î¹Ï‡Î¼Î¯Î¿Ï… Ï„Î¿Ï… ÏĴ±Ï„Î¿Ï, or deductive molecular mechanics of crystalline water. AIP Conference Proceedings, 2017, , .	0.2	3
83	cartesius fort - object fortran Library for Chemistry and Materials Science. Lecture Notes in Computer Science, 2019, , 639-651.	1.0	3
84	Deductive molecular mechanics of carbon allotropes (Review article). Low Temperature Physics, 2020, 46, 655-670.	0.2	3
85	Efficient magnetic superstructure optimization with ÎĴ¦. Computational Materials Science, 2021, 188, 110140.	1.4	3
86	The Effective Crystal Field Methodology as Used to Incorporate Transition Metals Into Molecular Mechanics. , 1997, , 217-232.		3
87	Electronic structure of karbin in the unrestricted Hartree-Fock approximation. Journal of Structural Chemistry, 1989, 30, 377-380.	0.3	2
88	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.	0.2	2
89	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.	0.4	2
90	Magneto-optical Response of 3d-Decorated Polyoxomolybdates with Îµ-Keggin Structure. Inorganic Chemistry, 2014, 53, 2892-2898.	1.9	2

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91	De glaciÄ“bus or deductive molecular mechanics of ice polymorphs. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	2
92	Minimum atomic parameter basis sets for elements 1â€“54 in a Hartreeâ€“Fock setting. International Journal of Quantum Chemistry, 2021, 121, e26687.	1.0	2
93	Synthesis, Characterization, and Quantum-Chemical Studies of Ni(CN)₂MX (M = Rb, Cs; X =) Tj ETQq1 1 0.784314 rgBT	1.9	1
94	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 spinâ€Hamiltonian models. International Journal of Quantum Chemistry, 2011, 111, 2490-2509.	1.0	1
95	The 13th V. A. Fock meeting on quantum and computational chemistry. International Journal of Quantum Chemistry, 2013, 113, 1813-1813.	1.0	1
96	Solidâ€state quantum chemistry with ÎˆÎ¦ (ThetaPhi): Spinâ€liquids , superconductors, and magnetic superstructures made computationally available. Journal of Computational Chemistry, 2021, 42, 1498-1513.	1.5	1
97	ÎÎµÏÎ¯ Ï„Î¿Ï… ÏƒÏ„Î¿Î¹Ï‡Î¼Î¯Î¿Ï… Ï„Î¿Ï… ÏÎ±Ï„Î¿Ï, or deductive molecular mechanics of crystalline water. , 0, .		1
98	Spin-Liquid States in a Copper-Based Material: The Mysterious Quantum Phase CuNCN. Quantum Matter, 2015, 4, 63-68.	0.2	1
99	Local perturbations of periodic systems. Chemisorption and point defects by GoGreenGo. Journal of Computational Chemistry, 2021, 42, 2352-2368.	1.5	1
100	Conductivity in quasiâ€oneâ€dimensional organic metals. A new approach. Journal of Chemical Physics, 1994, 100, 2223-2231.	1.2	0
101	Quantum mechanical models in catalysis. Russian Chemical Bulletin, 1996, 45, 505-510.	0.4	0
102	Physical Principles of Constructing Hybrid QM/MM Methods. Journal of Computational Methods in Sciences and Engineering, 2002, 2, 309-314.	0.1	0
103	Spatial distribution of atomic electronic density for elements 1â€“54 as coming from a Hartreeâ€“Fock treatment within the minimum atomic parameters paradigm. International Journal of Quantum Chemistry, 2021, 121, e26690.	1.0	0
104	Quantum Metrics for Continuous Shape Measures of Molecules. Russian Journal of Physical Chemistry A, 2021, 95, 1846-1856.	0.1	0
105	A theoretical simulation of the magnetic properties of nanocomposites based on graphene nanoflakes. International Journal of Quantum Chemistry, 2022, 122, .	1.0	0