Sergei F Vyboishchikov

List of Publications by Year
in descending order

54	2,427	249298	223390
papers	citations	26 h-index	49 g-index

56	56	56	2376
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A quick solvation energy estimator based on electronegativity equalization. Journal of Computational Chemistry, 2023, 44, 307-318.	1.5	4
2	Fast nonâ€iterative calculation of solvation energies for water and nonâ€aqueous solvents. Journal of Computational Chemistry, 2021, 42, 1184-1194.	1.5	21
3	Solvation Free Energies for Aqueous and Nonaqueous Solutions Computed Using PM7 Atomic Charges. Journal of Chemical Information and Modeling, 2021, 61, 4544-4553.	2.5	8
4	Fast and accurate calculation of hydration energies of molecules and ions. Physical Chemistry Chemical Physics, 2020, 22, 14591-14598.	1.3	36
5	A simple COSMO-based method for calculation of hydration energies of neutral molecules. Physical Chemistry Chemical Physics, 2019, 21, 18706-18713.	1.3	27
6	Sequential Oxidation and Câ^'H Bond Activation at a Gallium(I) Center. Angewandte Chemie - International Edition, 2019, 58, 18102-18107.	7.2	21
7	Sequential Oxidation and Câ^'H Bond Activation at a Gallium(I) Center. Angewandte Chemie, 2019, 131, 18270-18275.	1.6	6
8	Iterative Atomic Charge Partitioning of Valence Electron Density. Journal of Computational Chemistry, 2019, 40, 875-884.	1.5	18
9	A simple model for calculating atomic charges in molecules. Physical Chemistry Chemical Physics, 2018, 20, 23328-23337.	1.3	27
10	Unusual Reactions of NacNacAl with Urea and Phosphine Oxides. Inorganic Chemistry, 2017, 56, 5993-5997.	1.9	29
11	Oxidative Cleavage of the Câ•N Bond on Al(I). Journal of the American Chemical Society, 2017, 139, 8804-8807.	6.6	37
12	A Simple Local Correlation Energy Functional for Spherically Confined Atoms from ab Initio Correlation Energy Density. ChemPhysChem, 2017, 18, 3478-3484.	1.0	7
13	Correlation energy, correlated electron density, and exchange-correlation potential in some spherically confined atoms. Journal of Computational Chemistry, 2016, 37, 2677-2686.	1.5	6
14	Oxidative Cleavage of C=S and P=S Bonds at an Al^I Center: Preparation of Terminally Bound Aluminum Sulfides. Angewandte Chemie - International Edition, 2016, 55, 13306-13311.	7.2	61
15	Modeling exact exchange potential in spherically confined atoms. Journal of Computational Chemistry, 2015, 36, 2037-2043.	1.5	4
16	Serendipitous Metalâ€Catalyzed Hâ€"H/Siâ€"H Exchange. European Journal of Inorganic Chemistry, 2014, 2014, 2896-2901.	1.0	3
17	Dynamic Behavior of Hydrogen in Transition Metal Bis(silyl) Hydride Complexes. Organometallics, 2013, 32, 514-526.	1.1	7
18	Siâ‹…â‹…â‹…H Interligand Interactions in Cobalt(V) and Iridium(V) Bis(silyl)bis(hydride) Complexes. ChemPlusChem, 2013, 78, 1073-1081.	1.3	3

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19	Facile Activation of Hâ€“H and Siâ€“H Bonds by Boranes. Journal of the American Chemical Society, 2012, 134, 5488-5491.	6.6	73
20	A Hirshfeld Partitioning of the MP2 Correlation Energy: Method and Its Application to the Benzene Dimers. Journal of Chemical Theory and Computation, 2011, 7, 2049-2058.	2.3	4
21	Hydrogen Motion in Proton Sponge Cations: A Theoretical Study. ChemPhysChem, 2011, 12, 1118-1129.	1.0	18
22	Cationic Silane Ïƒ-Complexes of Ruthenium with Relevance to Catalysis. Journal of the American Chemical Society, 2010, 132, 5950-5951.	6.6	121
23	Properties of harmonium atoms from FCI calculations: Calibration and benchmarks for the ground state of the two-electron species. Physical Chemistry Chemical Physics, 2010, 12, 6712.	1.3	31
24	Mechanism for Hydride-Assisted Rearrangement from Ethylidene to Ethylene in Iridium Cationic Complexes. Organometallics, 2010, 29, 2040-2045.	1.1	28
25	Computational Study of Câ^'C Coupling on Diruthenium Bis(Î¼-vinyl) Ethylene Ï€-Complex. Organometallics, 2009, 28, 3029-3039.	1.1	7
26	Dynamics of Siâ^'Hâ^'Si Bridges in Agostically Stabilized Silylium Ions. Journal of Physical Chemistry A, 2009, 113, 1199-1209.	1.1	12
27	Partitioning of atomization energy. International Journal of Quantum Chemistry, 2008, 108, 708-718.	1.0	11
28	Computational Study of the Câ^'H Bond Activation in Ethylene on a Binuclear Ruthenium Complex. Organometallics, 2008, 27, 3681-3692.	1.1	8
29	Cp(Pr<i>‹sup›i‹/sup›‹/i›‹sub›2‹/sub›MeP)FeH‹sub›2‹/sub›SiR‹sub›3‹/sub›:â€‰ Nonclassical Iron Silyl Dihydride. Journal of the American Chemical Society, 2008, 130, 3732-3733.	6.6	97
30	Two complementary molecular energy decomposition schemes: The Mayer and Zieglerâ€“Rauk methods in comparison. Journal of Chemical Physics, 2008, 129, 144111.	1.2	19
31	Pseudopotential Calculations of Transition Metal Compounds: Scope and Limitations. Reviews in Computational Chemistry, 2007, , 63-144.	1.5	100
32	DFT Study of Hydride Exchange in a Binuclear Ruthenium Complex. Organometallics, 2007, 26, 56-64.	1.1	11
33	Rhodium Silyl Hydrides in Oxidation State +5:â€‰ Classical or Nonclassical?. Organometallics, 2007, 26, 4160-4169.	1.1	55
34	Persistent Silylium Ions Stabilized by Polyagostic Sïï£¿Hâ‹…â‹…â‹…Si Interactions. Angewandte Chemie - International Edition, 2007, 46, 4530-4533.	7.2	46
35	Ab initio energy partitioning at the correlated level. Chemical Physics Letters, 2006, 430, 204-209.	1.2	18
36	Unique {H(SiR3)2}, (H2SiR3), H(HSiR3), and (H2)SiR3 Ligand Sets Supported by the {Fe(Cp)(L)} Platform (L=CO, PR3). Chemistry - A European Journal, 2006, 12, 8518-8533.	1.7	28

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37	Chemical bonding in transition metal carbene complexes. Journal of Organometallic Chemistry, 2005, 690, 6178-6204.	0.8	206
38	Gas-phase reactions of V2O5+ and V2O6+ ions with CH3CF3 studied by density functional theory. Computational and Theoretical Chemistry, 2005, 723, 53-61.	1.5	8
39	Ring-Closing Olefin Metathesis on Ruthenium Carbene Complexes: Model DFT Study of Stereochemistry. Chemistry - A European Journal, 2005, 11, 3921-3935.	1.7	51
40	Density functional energy decomposition into one- and two-atom contributions. Journal of Chemical Physics, 2005, 122, 244110.	1.2	36
41	Cp*(iPr3P)Ru(Cl)(Î·2-HSiClMe2): the first complex with simultaneous Siâ€“H and RuClâ‹¯SiCl inter-ligand interactions. Chemical Communications, 2005, , 3349.	2.2	32
42	Versatile and Cooperative Reactivity of a Triruthenium Polyhydride Cluster. A Computational Study. Journal of the American Chemical Society, 2003, 125, 9910-9911.	6.6	25
43	Serendipitous syntheses and structures of [Cp2Nb(H){(SiMe2)2(Âµ-NR)}]Electronic supplementary information (ESI) available: experimental section. Fig. 1S and Table 1S. See http://www.rsc.org/suppdata/cc/b1/b111636c/ Dedicated to Prof. Dr J. Lorberth on the occasion of his 65th birthday.. Chemical Communications, 2002, , 568-569.	2.2	15
44	Mechanism of Olefin Metathesis with Catalysis by Ruthenium Carbene Complexes: Density Functional Studies on Model Systems. Chemistry - A European Journal, 2002, 8, 3962-3975.	1.7	182
45	(V2O5)n Gas-Phase Clusters (n = 1â^'12) Compared to V2O5 Crystal:â€‰ DFT Calculations. Journal of Physical Chemistry A, 2001, 105, 8588-8598.	1.1	135
46	Density Functional Study of Ethylene Polymerization Catalyzed by a Zirconium Non-Cyclopentadienyl Complex, L2ZrCH3+. Effects of Ligands and Bulky Substituents. Organometallics, 2001, 20, 309-323.	1.1	34
47	Gas-Phase Vanadium Oxide Anions:Â Structure and Detachment Energies from Density Functional Calculations. Journal of Physical Chemistry A, 2000, 104, 10913-10922.	1.1	110
48	Niobocene Silyl Hydride Complexes with Nonclassical Interligand Hypervalent Interactions. Chemistry - A European Journal, 1999, 5, 2947-2964.	1.7	60
49	Niobocene Silyl Hydride Complexes with Nonclassical Interligand Hypervalent Interactions. , 1999, 5, 2947.		1
50	Structure and Bonding of Low-Valent (Fischer-Type) and High-Valent (Schrock-Type) Transition Metal Carbene Complexes. Chemistry - A European Journal, 1998, 4, 1428-1438.	1.7	142
51	Transition Metal Coordinated Al(X)L2and Ga(X)L2Fragmentsâ€. Journal of the American Chemical Society, 1998, 120, 1237-1248.	6.6	114
52	Topological analysis of electron density distribution taken from a pseudopotential calculation. Journal of Computational Chemistry, 1997, 18, 416-429.	1.5	55
53	Structure and Bonding of the Transition-Metal Carbonyl Complexes M(CO)5L (M = Cr, Mo, W) and M(CO)3L (M = Ni, Pd, Pt; L = CO, SiO, CS, N2, NO+, CN-, NC-, HCCH, CCH2, CH2, CF2, H2)1. Organometallics, 1996, 15, 105-117.	1.1	193
54	Se₂NBr₃, Se₂NCl₅, Se₂NCl^{â€‹}₆: New Nitride Halides of Selenium(III) and Selenium(IV). Chemistry - A European Journal, 1996, 2, 1373-1378.	1.7	16