Wilhelm Hans Eugen Schwarz

List of Publications by Year
in descending order

40 papers	1,168 citations	361413 20 h-index	395702 33 g-index
44 all docs	44 docs citations	44 times ranked	1079 citing authors

#	Article	IF	Citations
1	The Lewis electron-pair bonding model: modern energy decomposition analysis. Nature Reviews Chemistry, 2019, 3, 48-63.	30.2	197
2	Measuring Orbitals: Provocation or Reality?. Angewandte Chemie - International Edition, 2006, 45, 1508-1517.	13.8	79
3	Uranyl-Glycine-Water Complexes in Solution: Comprehensive Computational Modeling of Coordination Geometries, Stabilization Energies, and Luminescence Properties. Inorganic Chemistry, 2011, 50, 2082-2093.	4.0	68
4	A diuranium carbide cluster stabilized inside a C80 fullerene cage. Nature Communications, 2018, 9, 2753.	12.8	63
5	Das Kombinierte Nï¿½herungsverfahren. Theoretica Chimica Acta, 1968, 11, 307-324.	0.8	59
6	The Lewis electron-pair bonding model: the physical background, one century later. Nature Reviews Chemistry, 2019, 3, 35-47.	30.2	52
7	On the maximum bond multiplicity of carbon: unusual Câ‰£U quadruple bonding in molecular CUO. Chemical Science, 2012, 3, 2786.	7.4	49
8	On the Upper Limits of Oxidation States in Chemistry. Angewandte Chemie - International Edition, 2018, 57, 3242-3245.	13.8	46
9	Nonspherical atomic groundâ€state densities and chemical deformation densities from xâ€ray scattering. Journal of Chemical Physics, 1990, 92, 4956-4969.	3.0	44
10	An 18-Electron System Containing a Superheavy Element: Theoretical Studies of Sg@Au₁₂. Inorganic Chemistry, 2015, 54, 3695-3701.	4.0	42
11	Theoretical Investigations of Geometry, Electronic Structure and Stability of UO₆: Octahedral Uranium Hexoxide and Its Isomers^{â€}. Journal of Physical Chemistry A, 2010, 114, 8837-8844.	2.5	39
12	Geometries, electronic structures, and excited states of UN2, NUO+, and UO 2 2+ : a combined CCSD(T), RAS/CASPT2 and TDDFT study. Theoretical Chemistry Accounts, 2011, 129, 467-481.	1.4	39
13	Bonding trends across the series of tricarbonato-actinyl anions [(AnO₂)(CO₃)₃]^{4â^’} (An = Uâ€“Cm): the plutonium turn. Dalton Transactions, 2017, 46, 2542-2550.	3.3	34
14	How Much Can Density Functional Approximations (DFA) Fail? The Extreme Case of the FeO₄ Species. Journal of Chemical Theory and Computation, 2016, 12, 1525-1533.	5.3	33
15	Understanding the Uniqueness of 2p Elements in Periodic Tables. Chemistry - A European Journal, 2020, 26, 15558-15564.	3.3	31
16	Probing the Electronic Structure and Chemical Bonding of Mono-Uranium Oxides with Different Oxidation States: UO_x^{â€“} and UO_x (x = 3â€“5). Journal of Physical Chemistry A, 2016, 120, 1084-1096.	2.5	29
17	Antibond Breakingâ€”The Formation and Decomposition of He@Adamantane: Descriptions, Explanations, and Meaning of Concepts. Chemistry - A European Journal, 2010, 16, 9107-9116.	3.3	27
18	Observations and Descriptions versus Explanationsâ€”An Example: Does Nature, Does Theory Know About Steric Hindrance?. Chemistry - A European Journal, 2012, 18, 4470-4479.	3.3	25

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19	On structure and bonding of lanthanoid trifluorides LnF3 (Ln = La to Lu). Physical Chemistry Chemical Physics, 2013, 15, 7839.	2.8	25
20	Theoretical Studies on Hexanuclear Oxometalates [M₆L₁₉]^{qâ"} (M = Cr, Mo, W, Sg, Nd, U). Electronic Structures, Oxidation States, Aromaticity, and Stability. Inorganic Chemistry, 2015, 54, 7171-7180.	4.0	24
21	Understanding Periodic and Non-periodic Chemistry in Periodic Tables. Frontiers in Chemistry, 2020, 8, 813.	3.6	22
22	Excited States and Absorption Spectra of UF₆: A RASPT2 Theoretical Study with Spinâ€"Orbit Coupling. Journal of Chemical Theory and Computation, 2011, 7, 3223-3231.	5.3	19
23	Physical origin of chemical periodicities in the system of elements. Pure and Applied Chemistry, 2019, 91, 1969-1999.	1.9	17
24	Ãœber Oxidationszahlâ€Obergrenzen in der Chemie. Angewandte Chemie, 2018, 130, 3297-3300.	2.0	15
25	Structures and stability of AnO₄ isomers, An = Pu, Am, and Cm: a relativistic density functional study. Physical Chemistry Chemical Physics, 2014, 16, 8997-9001.	2.8	13
26	100th Anniversary of Bohrâ€™s Model of the Atom. Angewandte Chemie - International Edition, 2013, 52, 12228-12238.	13.8	11
27	On Two Different Objectives of the Concepts of Ionic Radii. Chemistry - A European Journal, 2013, 19, 14758-14767.	3.3	11
28	Excited-State Chemistry: Photocatalytic Methanol Oxidation by Uranyl@Zeolite through Oxygen-Centered Radicals. Inorganic Chemistry, 2020, 59, 6287-6300.	4.0	11
29	Diversity of Chemical Bonding and Oxidation States in MS₄ Molecules of Groupâ€…8 Elements. Chemistry - A European Journal, 2017, 23, 10580-10589.	3.3	7
30	The Good Reasons for a Standard Periodic Table of the Chemical Elements. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2022, 648, .	1.2	4
31	Cis- and trans-binding influences in [NUOÂ·(N2)n]+. Journal of Chemical Physics, 2022, 157, .	3.0	4
32	Some solved problems of the periodic system of chemical elements. International Journal of Quantum Chemistry, 2009, 110, NA-NA.	2.0	3
33	Correspondence on â€œCore Electron Topologies in Chemical Compounds: Case Study of Carbon versus Siliconâ€• Angewandte Chemie, 2019, 131, 10512-10515.	2.0	3
34	Metal Oxo-Fluoride Molecules OnMF2 (M = Mn and Fe; n = 1â€"4) and O2MnF: Matrix Infrared Spectra and Quantum Chemistry. Inorganic Chemistry, 2021, 60, 7687-7696.	4.0	3
35	Electronic Structure and Spectroscopic Properties of Group-7 Tri-Oxo-Halides MO₃X (M =) Tj ETQq1 1 0.784314 rgBT /O	4.0	3
36	Correspondence on â€œCore Electron Topologies in Chemical Compounds: Case Study of Carbon versus Siliconâ€• Angewandte Chemie - International Edition, 2019, 58, 10404-10407.	13.8	2

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37	In memoriam Hermann Hartmann, founder of TCA, on the occasion of his 100th birthday. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	1
38	Editorial: Celebrating the International Year of the Periodic Table: Beyond Mendeleev 150. Frontiers in Chemistry, 2020, 8, 610869.	3.6	0
39	d- and s-orbital populations in the d block: unbound atoms in physical vacuum versus chemical elements in condensed matter. A Dronskowski-population analysis. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2021, 76, 547-557.	0.7	0
40	On the highest oxidation states of the actinoids in <scp> AnO ₄ </scp> molecules (AnÂ=ÂAc) Tj ETQq0 0 0 rgBT /Overlock	3.3	0