Marek Sierka

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1510805/publications.pdf

Version: 2024-02-01

118 papers	9,218 citations	41258 49 h-index	39575 94 g-index
137 all docs	137 docs citations	137 times ranked	8125 citing authors

#	Article	IF	Citations
1	Turbomole. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 91-100.	6.2	867
2	Fast evaluation of the Coulomb potential for electron densities using multipole accelerated resolution of identity approximation. Journal of Chemical Physics, 2003, 118, 9136-9148.	1.2	842
3	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	1.2	616
4	Application of semiempirical longâ€range dispersion corrections to periodic systems in density functional theory. Journal of Computational Chemistry, 2008, 29, 2088-2097.	1.5	294
5	Aluminum Siting in Siliconâ€Rich Zeolite Frameworks: A Combined Highâ€Resolution ²⁷Alâ€…NMR Spectroscopy and Quantum Mechanicsâ€‰/â€‰Molecular Mechanics Study of ZSMâ€5. Angewandte Chemie - International Edition, 2007, 46, 7286-7289.	7.2	234
6	Combining quantum mechanics and interatomic potential functions inab initio studies of extended systems. Journal of Computational Chemistry, 2000, 21, 1470-1493.	1.5	221
7	Coordination and siting of Cu+ ions in ZSM-5: A combined quantum mechanics/interatomic potential function study. Physical Chemistry Chemical Physics, 1999, 1, 2019-2026.	1.3	215
8	The Atomic Structure of a Metalâ€Supported Vitreous Thin Silica Film. Angewandte Chemie - International Edition, 2012, 51, 404-407.	7.2	207
9	Structure and reactivity of silica and zeolite catalysts by a combined quantum mechanics[ndash]shell-model potential approach based on DFT. Faraday Discussions, 1997, 106, 41-62.	1.6	203
10	Growth and Structure of Crystalline Silica Sheet on Ru(0001). Physical Review Letters, 2010, 105, 146104.	2.9	198
11	Aluminium siting in the ZSM-5 framework by combination of high resolution 27Al NMR and DFT/MM calculations. Physical Chemistry Chemical Physics, 2009, 11, 1237-1247.	1.3	196
12	Density functional study of palladium clusters. Physical Chemistry Chemical Physics, 2003, 5, 3372-3381.	1.3	171
13	Finding transition structures in extended systems: A strategy based on a combined quantum mechanicsâ€“empirical valence bond approach. Journal of Chemical Physics, 2000, 112, 6983-6996.	1.2	142
14	Proton Mobility in Chabazite, Faujasite, and ZSM-5 Zeolite Catalysts. Comparison Based on ab Initio Calculations. Journal of Physical Chemistry B, 2001, 105, 1603-1613.	1.2	132
15	Effect of Alâ€”Siâ€”Al and Alâ€”Siâ€”Siâ€”Al Pairs in the ZSM-5 Zeolite Framework on the ²⁷Al NMR Spectra. A Combined High-Resolution ²⁷Al NMR and DFT/MM Study. Journal of Physical Chemistry C, 2009, 113, 1447-1458.	1.5	121
16	Computational Elucidation of the Transition State Shape Selectivity Phenomenon. Journal of the American Chemical Society, 2004, 126, 936-947.	6.6	120
17	Unexpected Structures of Aluminum Oxide Clusters in the Gas Phase. Angewandte Chemie - International Edition, 2007, 46, 3372-3375.	7.2	113
18	Coordination of Cu+Ions to Zeolite Frameworks Strongly Enhances Their Ability To Bind NO2. An ab Initio Density Functional Study. Journal of the American Chemical Society, 1998, 120, 1545-1551.	6.6	109

#	Article	IF	Citations
19	Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, 10881-10905.	1.7	108
20	Thin silica films on Ru(0001): monolayer, bilayer and three-dimensional networks of [SiO4] tetrahedra. Physical Chemistry Chemical Physics, 2012, 14, 11344.	1.3	106
21	Heterogeneity of BrÃ¸nsted Acidic Sites in Faujasite Type Zeolites due to Aluminum Content and Framework Structure. Journal of Physical Chemistry B, 1998, 102, 6397-6404.	1.2	105
22	Structure determination of neutral MgO clustersâ€"hexagonal nanotubes and cages. Physical Chemistry Chemical Physics, 2012, 14, 2849.	1.3	100
23	Modeling Zeolites with Metalâ€Supported Twoâ€Dimensional Aluminosilicate Films. Angewandte Chemie - International Edition, 2012, 51, 6005-6008.	7.2	96
24	Stable Mechanistically-Relevant Aromatic-Based Carbenium Ions in Zeolite Catalysts. Journal of the American Chemical Society, 2003, 125, 2136-2141.	6.6	95
25	Stabilities of C3â€"C5 alkoxide species inside H-FER zeolite: a hybrid QM/MM study. Journal of Catalysis, 2005, 231, 393-404.	3.1	91
26	Nature of active sites in Ni2P hydrotreating catalysts as probed by iron substitution. Applied Catalysis B: Environmental, 2015, 164, 204-216.	10.8	91
27	Synergy between theory and experiment in structure resolution of low-dimensional oxides. Progress in Surface Science, 2010, 85, 398-434.	3.8	90
28	Point defects in CaF2 and CeO2 investigated by the periodic electrostatic embedded cluster method. Journal of Chemical Physics, 2009, 130, 174710.	1.2	88
29	Structures of the Ordered Water Monolayer on MgO(001). Journal of Physical Chemistry C, 2011, 115, 6764-6774.	1.5	88
30	Structures and Properties of Spherical 90â€Vertex Fullereneâ€Like Nanoballs. Chemistry - A European Journal, 2010, 16, 2092-2107.	1.7	87
31	Gas phase vibrational spectroscopy of mass-selected vanadium oxide anions. Physical Chemistry Chemical Physics, 2008, 10, 3992.	1.3	81
32	An Organometallic Nanosized Capsule Consisting of cycloâ€P₅ Units and Copper(I) Ions. Angewandte Chemie - International Edition, 2011, 50, 1435-1438.	7.2	79
33	One-Dimensional Polymers Based on [{CpMo(CO)2}2(?,?2-P2)]: Solid-State Conformation Analysis by NMR Spectroscopy and DFT Calculations. Chemistry - A European Journal, 2005, 11, 2163-2169.	1.7	75
34	Unprecedented selectivity to the direct desulfurization (DDS) pathway in a highly active FeNi bimetallic phosphide catalyst. Journal of Catalysis, 2012, 285, 1-5.	3.1	73
35	Translational proton motion in zeolite H-ZSM-5. Energy barriers and jump rates from DFT calculations. Physical Chemistry Chemical Physics, 2002, 4, 5207-5216.	1.3	71
36	The Complexed Triphosphaallyl Radical, Cation, and Anion Family. Angewandte Chemie - International Edition, 2009, 48, 2600-2604.	7.2	71

#	Article	IF	Citations
37	Resolution of identity approximation for the Coulomb term in molecular and periodic systems. Journal of Chemical Physics, 2009, 131, 214101.	1.2	68
38	Fixation and Release of Intact E₄ Tetrahedra (E=P, As). Angewandte Chemie - International Edition, 2015, 54, 4392-4396.	7.2	68
39	Structural Diversity and Flexibility of MgO Gasâ€Phase Clusters. Angewandte Chemie - International Edition, 2011, 50, 1716-1719.	7.2	67
40	Pnictogenâ€“Silicon Analogues of Benzene. Journal of the American Chemical Society, 2016, 138, 10433-10436.	6.6	62
41	Thickness-Dependent Hydroxylation of MgO(001) Thin Films. Journal of Physical Chemistry C, 2010, 114, 18207-18214.	1.5	57
42	Spherical Cluster Comprising a Four- and Six-Membered-Ring Motif. Angewandte Chemie - International Edition, 2006, 45, 2473-2475.	7.2	56
43	Physisorption and Chemisorption of Hydrocarbons in H-FAU Using QM-Pot(MP2//B3LYP) Calculations. Journal of Physical Chemistry C, 2008, 112, 11796-11812.	1.5	55
44	Intact As₄ Tetrahedra Coordinated Sideâ€On to Metal Cations. Angewandte Chemie - International Edition, 2013, 52, 858-861.	7.2	55
45	Unusual Coordination Behavior of P_nâ€Ligand Complexes with Tl⁺. Angewandte Chemie - International Edition, 2007, 46, 9323-9326.	7.2	52
46	Identification of Conical Structures in Small Aluminum Oxide Clusters: Infrared Spectroscopy of (Al₂O₃)_{1â^'4}(AlO)⁺. Journal of the American Chemical Society, 2008, 130, 15143-15149.	6.6	51
47	Reactions of H₂, CH₄, C₂H₆, and C₃H₈ with [(MgO)_n]⁺ Clusters Studied by Density Functional Theory. ChemCatChem, 2010, 2, 819-826.	1.8	51
48	Ultrathin Silica Films: The Atomic Structure of Twoâ€Dimensional Crystals and Glasses. Chemistry - A European Journal, 2014, 20, 9176-9183.	1.7	51
49	Structures and vibrational spectroscopy of partially reduced gas-phase cerium oxide clusters. Physical Chemistry Chemical Physics, 2011, 13, 19393.	1.3	50
50	Electron hole formation in acidic zeolite catalysts. Journal of Chemical Physics, 2004, 121, 6034-6041.	1.2	49
51	On the geometrical and electronic structure of an ultra-thin crystalline silica film grown on Mo(112). Surface Science, 2007, 601, 4849-4861.	0.8	48
52	Structure evolution of nanoparticulate Fe₂O₃. Nanoscale, 2015, 7, 2960-2969.	2.8	47
53	Synthesis and Structure of Ultrathin Aluminosilicate Films. Angewandte Chemie - International Edition, 2006, 45, 7636-7639.	7.2	45
54	Density Functional Theory for Molecular and Periodic Systems Using Density Fitting and Continuous Fast Multipole Methods. Journal of Chemical Theory and Computation, 2015, 11, 3029-3041.	2.3	45

#	Article	IF	Citations
55	Catalytic dehydrogenation of ethane over mononuclear Cr(III) surface sites on silica. part I. Câ€”H activation by Ïƒâ€bond metathesis. Journal of Physical Organic Chemistry, 2004, 17, 990-1006.	0.9	44
56	Access to Extended Polyphosphorus Frameworks. Angewandte Chemie - International Edition, 2010, 49, 6860-6864.	7.2	44
57	Complexes of Monocationic Groupâ€…13 Elements with Pentaphosphaâ€•and Pentaarsaferrocene. Chemistry - A European Journal, 2014, 20, 3759-3768.	1.7	44
58	Reaction pathways for growth of polycyclic aromatic hydrocarbons under combustion conditions, a DFT study. Physical Chemistry Chemical Physics, 2004, 6, 4377.	1.3	42
59	Electron Distribution in Partially Reduced Mixed Metal Oxide Systems: Infrared Spectroscopy of Ce_mV_nO_o⁺ Gas-Phase Clusters. Journal of Physical Chemistry A, 2011, 115, 11187-11192.	1.1	42
60	Tetraphosphacyclopentadienyl and Triphosphaallyl Ligands in Iron Complexes. Angewandte Chemie - International Edition, 2005, 44, 3755-3758.	7.2	40
61	The Potential of acyclo-As3-Ligand Complex in Supramolecular Chemistry. Angewandte Chemie - International Edition, 2006, 45, 4189-4192.	7.2	39
62	A Novel Soluble In^I Precursor for P_n Ligand Coordination Chemistry. Chemistry - A European Journal, 2010, 16, 13041-13045.	1.7	39
63	Fast atom diffraction during grazing scattering from a MgO(001) surface. Surface Science, 2012, 606, 161-173.	0.8	39
64	Oxygen adsorption on Mo(112) surface studied by ab initio genetic algorithm and experiment. Journal of Chemical Physics, 2007, 126, 234710.	1.2	37
65	Theoretical studies of Cu(i) sites in faujasite and their interaction with carbon monoxide. Physical Chemistry Chemical Physics, 2007, 9, 5446.	1.3	37
66	Linear Scaling Hierarchical Integration Scheme for the Exchange-Correlation Term in Molecular and Periodic Systems. Journal of Chemical Theory and Computation, 2011, 7, 3097-3104.	2.3	37
67	Conformational Analysis of One-Dimensional Coordination Polymers Based on [Cp2Cr2(CO)4(Î¼,Î·2-P2)] by Solid-State Multinuclear NMR Spectroscopy and Density Functional Calculations. European Journal of Inorganic Chemistry, 2007, 2007, 2775-2782.	1.0	35
68	Antimony-Tungsten Triple Bond: A Stable Complex with a Terminal Antimony Ligand. Angewandte Chemie - International Edition, 2005, 44, 4920-4924.	7.2	33
69	CdO and ZnO Clusters as Potential Building Blocks for Cluster-Assembled Materials: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry C, 2015, 119, 6886-6895.	1.5	31
70	Combined Quantum Mechanics:Â Interatomic Potential Function Investigation of rac-meso Configurational Stability and Rotational Transition in Zirconocene-Based Zieglerâ^'Natta Catalysts. Journal of Physical Chemistry A, 2000, 104, 10932-10938.	1.1	30
71	Density functional theory for molecular and periodic systems using density fitting and continuous fast multipole method: Analytical gradients. Journal of Computational Chemistry, 2016, 37, 2518-2526.	1.5	29
72	Acidic Catalysis by Zeolites: Ab Initio Modeling of Transition Structures. ACS Symposium Series, 1999, , 358-367.	0.5	27

#	Article	IF	Citations
73	Interplay between theory and experiment in the quest for silica with reduced dimensionality grown on a Mo(112) surface. Chemical Physics Letters, 2006, 424, 115-119.	1.2	27
74	The [(Al₂O₃)₂]^{â^'} Anion Cluster: Electron Localizationâ€“Delocalization Isomerism. ChemPhysChem, 2009, 10, 2410-2413.	1.0	27
75	Oneâ€Dimensional Polymers Based on Silver(I) Cations and Organometallic cycloâ€P₃ Ligand Complexes. Chemistry - an Asian Journal, 2009, 4, 1578-1587.	1.7	26
76	Control of the Crystal Phase Composition of Fe_xO_y Nanopowders Prepared by CO₂ Laser Vaporization. Crystal Growth and Design, 2013, 13, 4868-4876.	1.4	26
77	Formation of one-dimensional molybdenum oxide on Mo(112). Surface Science, 2008, 602, 3338-3342.	0.8	23
78	Different Reactivity of As₄ towards Disilenes and Silylenes. Angewandte Chemie - International Edition, 2017, 56, 6655-6659.	7.2	23
79	Effect of an electric field during the deposition of silicon dioxide thin films by plasma enhanced atomic layer deposition: an experimental and computational study. Nanoscale, 2020, 12, 2089-2102.	2.8	22
80	Molecular Alloys: Syntheses and Structures of the Copperâ^'Antimony Clusters [Cu17Sb8(dppm)6(Ph2PCHPPh2)] and [Cu20Sb10(PCy3)8]. European Journal of Inorganic Chemistry, 2004, 2004, 2933-2936.	1.0	21
81	Ab Initio energetics of Sï£¿O bond cleavage. Journal of Computational Chemistry, 2017, 38, 2349-2353.	1.5	21
82	Formation of one-dimensional crystalline silica on a metal substrate. Surface Science, 2006, 600, L164-L168.	0.8	19
83	Cage-Like Nanoclusters of ZnO Probed by Time-Resolved Photoelectron Spectroscopy and Theory. Journal of Physical Chemistry Letters, 2014, 5, 2642-2648.	2.1	19
84	Effects of ligand coverage on properties of palladium clusters. A density functional theory study. Physical Chemistry Chemical Physics, 2004, 6, 5338.	1.3	18
85	Vanadium Oxides Supported on a Thin Silica Film Grown on Mo(112): Insights from Density Functional Theory. Journal of Physical Chemistry C, 2009, 113, 8336-8342.	1.5	17
86	Similarity recognition of molecular structures by optimal atomic matching and rotational superposition. Journal of Computational Chemistry, 2012, 33, 134-140.	1.5	16
87	A Silica Bilayer Supported on Ru(0001): Following the Crystallineâ€to Vitreous Transformation in Real Time with Spectroâ€microscopy. Angewandte Chemie - International Edition, 2020, 59, 10587-10593.	7.2	15
88	The Complexed 1,3â€Diphosphaâ€2â€Arsaallyl Radical and Its Cationic and Anionic Derivatives. Chemistry - A European Journal, 2010, 16, 7488-7495.	1.7	14
89	Structure and properties of bimetallic titanium and vanadium oxide clusters. Physical Chemistry Chemical Physics, 2014, 16, 8441.	1.3	13
90	Kinetics of Decelerated Melting. Advanced Science, 2018, 5, 1700850.	5.6	13

#	Article	IF	Citations
91	Modeling environmental effects on charge density distributions in polar organometallics: Validation of embedded cluster models for the methyl lithium crystal. Journal of Computational Chemistry, 2010, 31, 2568-2576.	1.5	12
92	Thermodynamic compatibility of actives encapsulated into PEGâ€PLA nanoparticles: In Silico predictions and experimental verification. Journal of Computational Chemistry, 2016, 37, 2220-2227.	1.5	12
93	Block Copolymers Composed of PEtOx and Polyesteramides Based on Glycolic Acid, <scp>l</scp>-Valine, and <scp>l</scp>-Isoleucine. Macromolecules, 2020, 53, 3580-3590.	2.2	12
94	Predicting Solubility of Small Molecules in Macromolecular Compounds for Nanomedicine Application from Atomistic Simulations. Advanced Theory and Simulations, 2020, 3, 2000001.	1.3	11
95	Template Synthesis and Theoretical Investigation of[CuII2CuI3K6(Î¼6-Cl)(Î¼3-OtBu)12]: The First Mixed-Valence Copper Alkoxide. Angewandte Chemie - International Edition, 2003, 42, 4036-4039.	7.2	10
96	WO₃ as a nucleating agent for BaO/SrO/ZnO/SiO₂ glasses â€“ experiments and simulations. CrystEngComm, 2018, 20, 4565-4574.	1.3	10
97	Realâ€time timeâ€dependent density functional theory using density fitting and the continuous fast multipole method. Journal of Computational Chemistry, 2020, 41, 2573-2582.	1.5	10
98	Structure Prediction of Rare Earth Doped BaO and MgO Containing Aluminosilicate Glassesâ€“the Model Case of Gd2O3. Materials, 2018, 11, 1790.	1.3	9
99	Atomistic Simulations of Plasma-Enhanced Atomic Layer Deposition. Materials, 2019, 12, 2605.	1.3	9
100	A polyesteramide library from dicarboxylic acids and 2,2â€²-bis(2-oxazoline): synthesis, characterization, nanoparticle formulation and molecular dynamics simulations. Polymer Chemistry, 2020, 11, 112-124.	1.9	9
101	A combined experimental and in silico approach to determine the compatibility of poly(ester amide)s and indomethacin in polymer nanoparticles. European Polymer Journal, 2021, 156, 110606.	2.6	9
102	Parametrization in Models of Subcritical Glass Fracture: Activation Offset and Concerted Activation. Frontiers in Materials, 2017, 4, .	1.2	8
103	Hybrid Quantum Mechanics/ Molecular Mechanics Methods and their Application. , 2005, , 241-258.		8
104	Dynamics of ultrathin gold layers on vitreous silica probed by density functional theory. Physical Chemistry Chemical Physics, 2015, 17, 27488-27495.	1.3	7
105	Effect of Al2O3 on phase formation and thermal expansion of a BaO-SrO-ZnO-SiO2 glass ceramic. Ceramics International, 2018, 44, 2098-2108.	2.3	7
106	The Structure of Gd3+-Doped Li2O and K2O Containing Aluminosilicate Glasses from Molecular Dynamics Simulations. Materials, 2021, 14, 3265.	1.3	7
107	Density functional theory for molecular and periodic systems using density fitting and continuous fast multipole method: Stress tensor. Journal of Computational Chemistry, 2019, 40, 2563-2570.	1.5	6
108	Palladium speciation in UVâ€transparent glasses. Journal of the American Ceramic Society, 2020, 103, 4214-4223.	1.9	5

#	Article	IF	Citations
109	Aluminum siting in the framework of silicon rich zeolites. A ZSM-5 study. Studies in Surface Science and Catalysis, 2008, , 781-786.	1.5	4
110	Unterschiedliche ReaktivitÃt von As₄ gegenÃ¼ber Disilenen und Silylenen. Angewandte Chemie, 2017, 129, 6755-6759.	1.6	4
111	A Silica Bilayer Supported on Ru(0001): Following the Crystallineâ€to Vitreous Transformation in Real Time with Spectroâ€microscopy. Angewandte Chemie, 2020, 132, 10674-10680.	1.6	4
112	Atomistic Descriptors for Machine Learning Models of Solubility Parameters for Small Molecules and Polymers. Polymers, 2022, 14, 26.	2.0	4
113	Relative stability of alkoxides and carbocations in zeolites. QM/MM embedding and QM calculations applying periodic boundary conditions. Studies in Surface Science and Catalysis, 2002, 142, 643-649.	1.5	3
114	Thermomechanical properties of zero thermal expansion materials from theory and experiments. Physical Chemistry Chemical Physics, 2020, 22, 18518-18525.	1.3	3
115	Tunable phase stability of negative thermal expansion materials by theory and experiment. Physical Chemistry Chemical Physics, 2021, 23, 25533-25541.	1.3	1
116	Density Functional Study of Palladium Clusters. ChemInform, 2003, 34, no.	0.1	0
117	Structure and crystallization of SiO₂and B₂O₃doped lithium disilicate glasses from theory and experiment. Physical Chemistry Chemical Physics, 2017, 19, 25298-25308.	1.3	0
118	Hans-Joachim Freund and Joachim Sauer Preface. Journal of Physical Chemistry C, 2019, 123, 7495-7498.	1.5	0