Notker RÃ¶sch

List of Publications by Year
in descending order

177 papers	6,781 citations	50244 46 h-index	74108 75 g-index
181 all docs	181 docs citations	181 times ranked	5423 citing authors

#	Article	IF	Citations
1	From clusters to bulk: A relativistic density functional investigation on a series of gold clusters Aun, n=6,â€¦,147. Journal of Chemical Physics, 1997, 106, 5189-5201.	1.2	340
2	Fragment charge difference method for estimating donorâ€“acceptor electronic coupling: Application to DNA Ï€-stacks. Journal of Chemical Physics, 2002, 117, 5607-5616.	1.2	294
3	CO Adsorption on Pd Nanoparticles:Â Density Functional and Vibrational Spectroscopy Studies. Journal of Physical Chemistry B, 2003, 107, 255-264.	1.2	262
4	A scalar-relativistic extension of the linear combination of Gaussian-type orbitals local density functional method: application to AuH, AuCl and Au2. Chemical Physics Letters, 1992, 199, 491-496.	1.2	181
5	Comment on â€œConcerning the applicability of density functional methods to atomic and molecular negative ionsâ€•[J. Chem. Phys. 105, 862 (1996)]. Journal of Chemical Physics, 1997, 106, 8940-8941.	1.2	177
6	Density functional study of small molecules and transition-metal carbonyls using revised PBE functionals. International Journal of Quantum Chemistry, 1999, 75, 863-873.	1.0	164
7	Site preference of CO chemisorbed on Pt(111) from density functional calculations. Surface Science, 2003, 530, 71-87.	0.8	155
8	Size Dependence of the Adsorption Energy of CO on Metal Nanoparticles: A DFT Search for the Minimum Value. Nano Letters, 2012, 12, 2134-2139.	4.5	155
9	Metal nanoparticles as models of single crystal surfaces and supported catalysts: Density functional study of size effects for CO/Pd(111). Journal of Chemical Physics, 2002, 117, 9887-9896.	1.2	144
10	Olefin Epoxidation with Inorganic Peroxides. Solutions to Four Long-Standing Controversies on the Mechanism of Oxygen Transfer. Accounts of Chemical Research, 2004, 37, 645-652.	7.6	142
11	Density functional based structure optimization for molecules containing heavy elements: analytical energy gradients for the Douglas-Kroll-Hess scalar relativistic approach to the LCGTO-DF method. Chemical Physics, 1996, 210, 413-425.	0.9	127
12	Trigonal-Bipyramidal Lewis Base Adducts of Methyltrioxorhenium(VII) and Their Bisperoxo Congeners: Characterization, Application in Catalytic Epoxidation, and Density Functional Mechanistic Study. Chemistry - A European Journal, 1999, 5, 3603-3615.	1.7	122
13	Cluster embedding in an elastic polarizable environment: Density functional study of Pd atoms adsorbed at oxygen vacancies of MgO(001). Journal of Chemical Physics, 2001, 115, 8157-8171.	1.2	116
14	The average bond length in Pd clusters Pdn, n=4â€“309: A density-functional case study on the scaling of cluster properties. Journal of Chemical Physics, 2001, 115, 2082-2087.	1.2	110
15	Oxidation of Supported Rhodium Clusters by Support Hydroxy Groups. Angewandte Chemie - International Edition, 2003, 42, 1391-1394.	7.2	107
16	Density functional study of Pd nanoparticles with subsurface impurities of light element atoms. Physical Chemistry Chemical Physics, 2004, 6, 116-123.	1.3	105
17	Hydrodeoxygenation of Guaiacol over Ru(0001): A DFT Study. ACS Catalysis, 2014, 4, 4178-4188.	5.5	105
18	Relativistic effects in the electronic structure of the monoxides and monocarbonyls of Ni, Pd, and Pt: Local and gradientâ€corrected density functional calculations. Journal of Chemical Physics, 1995, 102, 3695-3702.	1.2	96

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19	Variational fitting methods for electronic structure calculations. Molecular Physics, 2010, 108, 3167-3180.	0.8	89
20	A two-component variant of the Douglasâ€“Kroll relativistic linear combination of Gaussian-type orbitals density-functional method: Spinâ€“orbit effects in atoms and diatomics. Journal of Chemical Physics, 2001, 115, 4411-4423.	1.2	86
21	Size-Dependence of Adsorption Properties of Metal Nanoparticles: A Density Functional Study on Palladium Nanoclusters. Journal of Physical Chemistry C, 2008, 112, 20269-20275.	1.5	86
22	Optical Absorption Spectrum of Gold Atoms Deposited onSiO2from Cavity Ringdown Spectroscopy. Physical Review Letters, 2005, 94, 213402.	2.9	80
23	How the Câ”O Bond Breaks during Methanol Decomposition on Nanocrystallites of Palladium Catalysts. Journal of the American Chemical Society, 2008, 130, 9342-9352.	6.6	77
24	Ethylidyne Formation from Ethylene over Pt(111): A Mechanistic Study from First-Principle Calculations. Journal of Physical Chemistry C, 2010, 114, 12190-12201.	1.5	77
25	Particle-size dependent heats of adsorption of CO on supported Pd nanoparticles as measured with a single-crystal microcalorimeter. Physical Review B, 2010, 81, .	1.1	77
26	Faujasite-Supported Ir4Clusters:Â A Density Functional Model Study of Metalâ”Zeolite Interactions. Journal of Physical Chemistry B, 1999, 103, 5311-5319.	1.2	75
27	Elastic Polarizable Environment Cluster Embedding Approach for Covalent Oxides and Zeolites Based on a Density Functional Method. Journal of Physical Chemistry B, 2003, 107, 2228-2241.	1.2	73
28	Olefin Epoxidation by Methyltrioxorhenium: A Density Functional Study on Energetics and Mechanisms. Angewandte Chemie - International Edition, 1998, 37, 2211-2214.	7.2	70
29	Comparative study of relativistic density functional methods applied to actinide species AcO22+and AcF6for Ac = U, Np. Journal of Computational Chemistry, 2002, 23, 834-846.	1.5	67
30	Ethylene conversion to ethylidyne on Pd(111) and Pt(111): A first-principles-based kinetic Monte Carlo study. Journal of Catalysis, 2012, 285, 187-195.	3.1	66
31	Role of Solvation in the Reduction of the Uranyl Dication by Water:Â A Density Functional Study. Inorganic Chemistry, 2004, 43, 4080-4090.	1.9	65
32	On the evolution of cluster to bulk properties: a theoretical LCGTO-LDF study of free and coordinated Nin clusters (n=6-147). Chemical Physics, 1994, 184, 125-137.	0.9	61
33	Computational Study of Model Pdâ”Zn Nanoclusters and Their Adsorption Complexes with CO Molecules. Journal of Physical Chemistry B, 2004, 108, 5424-5430.	1.2	59
34	Reverse Hydrogen Spillover onto Zeolite-Supported Metal Clusters:â€‰ An Embedded Cluster Density Functional Study of Models M₆(M = Rh, Ir, or Au). Journal of Physical Chemistry C, 2007, 111, 12340-12351.	1.5	57
35	Relativistic density-functional studies of naked and ligated gold clusters. International Journal of Quantum Chemistry, 1994, 52, 595-610.	1.0	56
36	Ethylene Conversion to Ethylidyne over Pd(111): Revisiting the Mechanism with First-Principles Calculations. Journal of Physical Chemistry C, 2009, 113, 2512-2520.	1.5	56

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37	Size dependence of bond length and binding energy in palladium and gold clusters. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1997, 101, 1640-1643.	0.9	55
38	Adsorption of dimers and trimers of Cu, Ag, and Au on regular sites and oxygen vacancies of the MgO(001) surface: a density functional study using embedded cluster models. Applied Physics A: Materials Science and Processing, 2006, 82, 181-189.	1.1	52
39	Decomposition of ethylene on transition metal surfaces M(111). A comparative DFT study of model reactions for M=Pd, Pt, Rh, Ni. Journal of Molecular Catalysis A, 2011, 344, 37-46.	4.8	52
40	Reverse hydrogen spillover in supported subnanosize clusters of the metals of groups 8 to 11. A computational model study. Physical Chemistry Chemical Physics, 2005, 7, 4019.	1.3	51
41	A Density Functional Study of Uranyl Monocarboxylates. Inorganic Chemistry, 2006, 45, 1480-1490.	1.9	51
42	Allylic Alcohol Epoxidation by Methyltrioxorhenium: A Density Functional Study on the Mechanism and the Role of Hydrogen Bonding. Journal of the American Chemical Society, 2001, 123, 2365-2376.	6.6	49
43	The hydration of the uranyl dication: Incorporation of solvent effects in parallel density functional calculations with the program PARAGAUSS. International Journal of Quantum Chemistry, 2002, 86, 487-501.	1.0	47
44	Gold Atoms and Dimers on Amorphous SiO2:Â Calculation of Optical Properties and Cavity Ringdown Spectroscopy Measurements. Journal of Physical Chemistry B, 2005, 109, 19876-19884.	1.2	47
45	Mechanism of Selective Hydrogenation of Î±,Î²-Unsaturated Aldehydes on Silver Catalysts: A Density Functional Study. Journal of Physical Chemistry C, 2009, 113, 13231-13240.	1.5	47
46	Transformations of Ethylene on the Pd(111) Surface: A Density Functional Study. Journal of Physical Chemistry C, 2010, 114, 17683-17692.	1.5	47
47	Activation of Hydrogen Peroxide by Ionic Liquids: Mechanistic Studies and Application in the Epoxidation of Olefins. Chemistry - A European Journal, 2013, 19, 5972-5979.	1.7	47
48	Hydrogen Activation on Silver:â€‰ A Computational Study on Surface and Subsurface Oxygen Species. Journal of Physical Chemistry C, 2008, 112, 1628-1635.	1.5	44
49	A computational study of H2dissociation on silver surfaces: The effect of oxygen in the added row structure of Ag(110). Physical Chemistry Chemical Physics, 2007, 9, 1247-1254.	1.3	43
50	Systematic DFT Study of Gas Phase and Solvated Uranyl and Neptunyl Complexes [AnO2X4]n(An = U, Np;) Tj ETQq0 0 0 rgBT /Overlock	1.9	41
51	DFT Studies of Palladium Model Catalysts: Structure and Size Effects. Journal of Cluster Science, 2011, 22, 433-448.	1.7	39
52	Size-Dependence of the Adsorption Energy of CO on Pt Nanoparticles: Tracing Two Intersecting Trends by DFT Calculations. Journal of Physical Chemistry C, 2017, 121, 17371-17377.	1.5	39
53	Tuning the selectivity for ring-opening reactions of methylcyclopentane over Pt catalysts: A mechanistic study from first-principles calculations. Journal of Catalysis, 2012, 285, 124-133.	3.1	38
54	Small Platinum Clusters in Zeolites:Â A Density Functional Study of CO Adsorption on Electronically Modified Models. Journal of Physical Chemistry B, 1999, 103, 216-226.	1.2	36

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55	The cluster Ir4 and its interaction with a hydrogen impurity. A density functional study. Physical Chemistry Chemical Physics, 2005, 7, 2656.	1.3	36
56	Effects of the Aluminum Content of a Zeolite Framework:â€‰ A DFT/MM Hybrid Approach Based on Cluster Models Embedded in an Elastic Polarizable Environment. Journal of Chemical Theory and Computation, 2005, 1, 459-471.	2.3	36
57	Decomposition of Ethanol Over Ru(0001): A DFT Study. Topics in Catalysis, 2013, 56, 874-884.	1.3	36
58	Adsorption of carbon on Pd clusters of nanometer size: A first-principles theoretical study. Journal of Chemical Physics, 2005, 122, 174705.	1.2	33
59	Adsorption of Cu4, Ag4 and Au4 particles on the regular MgO(001) surface: A density functional study using embedded cluster models. Chemical Physics Letters, 2006, 417, 515-520.	1.2	33
60	Ring-Opening Reactions of Methylcyclopentane over Metal Catalysts, M = Pt, Rh, Ir, and Pd: A Mechanistic Study from First-Principles Calculations. ACS Catalysis, 2013, 3, 196-205.	5.5	33
61	Quantum chemistry with the Douglas-Kroll-Hess approach to relativistic density functional theory: Efficient methods for molecules and materials. Theoretical and Computational Chemistry, 2004, 14, 656-722.	0.2	32
62	Predicting adsorption enthalpies on silicalite and HZSMâ€5: A benchmark study on DFT strategies addressing dispersion interactions. Journal of Computational Chemistry, 2014, 35, 809-819.	1.5	31
63	Density functional modeling of reverse hydrogen spillover on zeolite-supported tetrairidium clusters. Chemical Physics Letters, 2007, 444, 215-219.	1.2	30
64	Ethylidyne Formation from Ethylene over Pd(111): Alternative Routes from a Density Functional Study. Journal of Physical Chemistry C, 2009, 113, 15373-15379.	1.5	29
65	Hydrogen adsorption on and spillover from Au- and Cu-supported Pt3 and Pd3 clusters: a density functional study. Physical Chemistry Chemical Physics, 2012, 14, 16062.	1.3	28
66	Metalâ€Free Polymerization of Phenylsilane: Tris(pentafluorophenyl)boraneâ€Catalyzed Synthesis of Branched Polysilanes at Elevated Temperatures. Chemistry - A European Journal, 2013, 19, 12526-12536.	1.7	28
67	Linear response formalism for the Douglasâ€“Krollâ€“Hess approach to the Diracâ€“Kohnâ€“Sham problem: Firstâ€•and secondâ€•order nuclear displacement derivatives of the energy. International Journal of Quantum Chemistry, 2007, 107, 3236-3249.	1.0	27
68	Theoretical study of carbon species on Pd(111): competition between migration of C atoms to the subsurface interlayer and formation of Cn clusters on the surface. Physical Chemistry Chemical Physics, 2009, 11, 10955.	1.3	27
69	Saturation of Small Supported Metal Clusters by Adsorbed Hydrogen. A Computational Study on Tetrahedral Models of Rh₄, Ir₄, and Pt₄. Journal of Physical Chemistry C, 2010, 114, 8500-8506.	1.5	27
70	Palladium-Catalyzed Hydroxycarbonylation of Pentenoic Acids. Computational and Experimental Studies on the Catalytic Selectivity. ACS Catalysis, 2017, 7, 7070-7080.	5.5	27
71	Free and Zeolite-Supported Hexarhodium Clusters with Light Impurity Atoms. Journal of Physical Chemistry B, 2004, 108, 180-192.	1.2	26
72	Câ€“O cleavage of aromatic oxygenates over ruthenium catalysts. A computational study of reactions at step sites. Physical Chemistry Chemical Physics, 2015, 17, 15324-15330.	1.3	26

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73	Modeling Polaron-Coupled Li Cation Diffusion in V₂O₅ Cathode Material. Journal of Physical Chemistry C, 2018, 122, 150-157.	1.5	26
74	Adsorption of acrolein on single-crystal surfaces of silver: Density functional studies. Chemical Physics Letters, 2006, 420, 60-64.	1.2	25
75	Density Functional Study of Hydrogen Adsorption on Tetrairidium Supported on Hydroxylated and Dehydroxylated Zeolite Surfaces. Journal of Physical Chemistry C, 2007, 111, 14484-14492.	1.5	25
76	Câ€“O bond scission of methoxide on Pd nanoparticles: A density functional study. Physical Chemistry Chemical Physics, 2006, 8, 2396-2401.	1.3	24
77	Spinâ€“orbit interaction in the Douglasâ€“Kroll approach to relativistic density functional theory: the screened nuclear potential approximation for molecules. Chemical Physics Letters, 2003, 382, 186-193.	1.2	23
78	Improving Upon String Methods for Transition State Discovery. Journal of Chemical Theory and Computation, 2012, 8, 777-786.	2.3	23
79	Density Functional Embedded Cluster Study of Cu4, Ag4and Au4Species Interacting with Oxygen Vacancies on the MgO(001) Surface. Chemistry - A European Journal, 2007, 13, 277-286.	1.7	22
80	Modeling metal adsorption at amorphous silica: Gold atoms and dimers as example. Chemical Physics Letters, 2007, 444, 280-286.	1.2	22
81	Atomic approximation to the projection on electronic states in the Douglas-Kroll-Hess approach to the relativistic Kohn-Sham method. Journal of Chemical Physics, 2008, 128, 244102.	1.2	22
82	Uranyl monocarboxylates of aromatic acids: A density functional model study of uranyl humate complexation. Dalton Transactions, 2009, , 3590.	1.6	22
83	Structure of Pd/Au Alloy Nanoparticles from a Density Functional Theory-Based Embedded-Atom Potential. Journal of Physical Chemistry C, 2013, 117, 21810-21822.	1.5	22
84	Structure, stability, electronic and magnetic properties of Ni4 clusters containing impurity atoms. Physical Chemistry Chemical Physics, 2006, 8, 1282.	1.3	21
85	First Hybrid Embedding Scheme for Polar Covalent Materials Using an Extended Border Region To Minimize Boundary Effects on the Quantum Region. Journal of Chemical Theory and Computation, 2007, 3, 2290-2300.	2.3	21
86	Hybrid Density Functionals for Clusters of Late Transition Metals: Assessing Energetic and Structural Properties. Journal of Chemical Theory and Computation, 2014, 10, 4408-4416.	2.3	21
87	Structure and electronic properties of MoVO type mixed-metal oxides â€“ a combined view by experiment and theory. Dalton Transactions, 2015, 44, 13778-13795.	1.6	21
88	The DFT+U method in the linear combination of Gaussian-type orbitals framework: Role of 4f orbitals in the bonding of LuF3. Chemical Physics Letters, 2009, 468, 158-161.	1.2	20
89	Scalable properties of metal clusters: A comparative study of modern exchange-correlation functionals. Journal of Chemical Physics, 2012, 137, 034102.	1.2	20
90	Photofragments of Ni(CO)4: A linear combination of Gaussianâ€type orbitals (LCGTO) XÎ± study. Journal of Chemical Physics, 1987, 86, 4038-4045.	1.2	19

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91	On the metallic droplet model for successive ionization potentials of metal clusters â€•relativistic electronic structure investigations of the icosahedral gold cluster Au₅₅. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1994, 98, 882-885.	0.9	19
92	Density functional embedded cluster calculations on Lewis acid centers of the Î±-Al2O3(0001) surface: Adsorption of a CO probe. International Journal of Quantum Chemistry, 2002, 90, 386-402.	1.0	19
93	Two hydrogen ligands on tetrairidium clusters: a relativistic density functional study. Physical Chemistry Chemical Physics, 2006, 8, 3391-3398.	1.3	19
94	Efficient symmetry treatment for the nonrelativistic and relativistic molecular Kohnâ€“Sham problem. The symmetry module of the program ParaGauss. Computer Physics Communications, 2004, 160, 91-119.	3.0	18
95	Hydrogen Adsorption on Zeolite-Supported Tetrairidium Clusters. Thermodynamic Modeling from Density Functional Calculations. Journal of Physical Chemistry C, 2008, 112, 18572-18577.	1.5	18
96	Theoretical study on the leaching of palladium in a CO atmosphere. Catalysis Science and Technology, 2012, 2, 2238.	2.1	18
97	Reverse hydrogen spillover on and hydrogenation of supported metal clusters: insights from computational model studies. Physical Chemistry Chemical Physics, 2012, 14, 5879.	1.3	18
98	Toward a Reliable Energetics of Adsorption at Solvated Mineral Surfaces: A Computational Study of Uranyl(VI) on 2:1 Clay Minerals. Journal of Physical Chemistry C, 2016, 120, 324-335.	1.5	18
99	Ethene hydrogenation vs. dimerization over a faujasite-supported [Rh(C₂H₄)₂] complex. A computational study of mechanism. Catalysis Science and Technology, 2017, 7, 102-113.	2.1	18
100	The Heat of Formation of the Uranyl Dication: Theoretical Evaluation Based on Relativistic Density Functional Calculations. Chemistry - A European Journal, 2006, 12, 629-634.	1.7	17
101	Modeling Catalytic Steps on Extra-Framework Metal Centers in Zeolites. A Case Study on Ethylene Dimerization. Journal of Physical Chemistry C, 2014, 118, 25077-25088.	1.5	16
102	Assessment of Hybrid Density Functionals for the Adsorption of Carbon Monoxide on Platinum Model Clusters. Journal of Physical Chemistry A, 2015, 119, 4051-4056.	1.1	16
103	Size-dependent properties of transition metal clusters: from molecules to crystals and surfaces â€“ computational studies with the program ParaGauss. Physical Chemistry Chemical Physics, 2015, 17, 28463-28483.	1.3	16
104	The origin of the particle-size-dependent selectivity in 1-butene isomerization and hydrogenation on Pd/Al2O3 catalysts. Nature Communications, 2021, 12, 6098.	5.8	16
105	Comparative density functional study of the complexes [UO2(CO3)3]4â^' and [(UO2)3(CO3)6]6â^' in aqueous solution. Dalton Transactions, 2010, 39, 5705.	1.6	15
106	Electronic and magnetic properties of organometallic clusters: From the molecular to the metallic state. International Journal of Quantum Chemistry, 1992, 44, 605-619.	1.0	14
107	Role of aliphatic and phenolic hydroxyl groups in uranyl complexation by humic substances. Inorganica Chimica Acta, 2009, 362, 2542-2550.	1.2	14
108	Transformations of Organic Molecules over Metal Surfaces: Insights from Computational Catalysis. Chemical Record, 2016, 16, 2388-2404.	2.9	14

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109	Ethene Dimerization and Hydrogenation over a Zeolite-Supported Rh(I)-Carbonyl Complex: Mechanistic Insights from DFT Modeling. ACS Catalysis, 2018, 8, 9836-9846.	5.5	14
110	Catalytic Transformations of 1-Butene over Palladium. A Combined Experimental and Theoretical Study. ACS Catalysis, 2018, 8, 5675-5685.	5.5	14
111	The heat of formation of gaseous PuO22+from relativistic density functional calculations. Physical Chemistry Chemical Physics, 2006, 8, 3767-3773.	1.3	13
112	Comment on â€œTowards understanding the bifunctional hydrodeoxygenation and aqueous phase reforming of glycerolâ€•[J. Catal. 269 (2010) 411â€“420]. Journal of Catalysis, 2012, 287, 210-213.	3.1	13
113	Hydrogen Adsorption on Small Zeolite-Supported Rhodium Clusters. A Density Functional Study. Journal of Physical Chemistry C, 2015, 119, 1121-1129.	1.5	13
114	Acrolein oxidation to acrylic acid over the MoVOx material. Insights from DFT modeling. Applied Catalysis A: General, 2018, 565, 68-75.	2.2	13
115	Impurity Effects on Small Pd Clusters: A Relativistic Density Functional Study of Pd4X, X = H, C, O. Journal of Physical Chemistry A, 2008, 112, 7739-7744.	1.1	12
116	Effects of the self-interaction error in Kohnâ€“Sham calculations: A DFT+U case study on penta-aqua uranyl(VI). Computational and Theoretical Chemistry, 2011, 963, 337-343.	1.1	12
117	Metal-Supported Metal Clusters: A Density Functional Study of Pt₃ and Pd₃. Journal of Physical Chemistry C, 2012, 116, 10057-10063.	1.5	12
118	Interaction of silica-supported small silver clusters with molecular oxygen. A computational study. Surface Science, 2014, 630, 265-272.	0.8	12
119	The IMOMM (Integrated Molecular Orbitals/Molecular Mechanics) Approach for Ligand-Stabilized Metal Clusters. Comparison to Full Density Functional Calculations for the Model Thiolate Cluster Cu13(SCH2CH3)8. Journal of Chemical Theory and Computation, 2006, 2, 47-58.	2.3	11
120	Ternary uranyl hydroxo acetate complexes: A computational study of structure, energetics, and stability constants. Inorganica Chimica Acta, 2010, 363, 263-269.	1.2	11
121	Carbon Dioxide Insertion into Diamines: A Computational Study of Solvent Effects. ChemSusChem, 2012, 5, 1967-1973.	3.6	11
122	Evaluation of density functionals for elementary steps of selective oxidation reactions. Computational and Theoretical Chemistry, 2017, 1101, 36-45.	1.1	11
123	CO2 reduction by H2 to CHO on Ru(0001): DFT evaluation of three pathways. Surface Science, 2019, 681, 54-58.	0.8	11
124	Mechanism of Olefin Epoxidation by Transition Metal Peroxo Compounds. Catalysis By Metal Complexes, 2002, , 289-324.	0.6	10
125	Influence of Single Impurity Atoms on the Structure, Electronic, and Magnetic Properties of Ni5 Clusters. Journal of Physical Chemistry A, 2007, 111, 2067-2076.	1.1	10
126	Density functional study of Ni6 clusters containing impurity atoms. Chemical Physics, 2008, 348, 61-68.	0.9	10

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127	Small gold species supported on alumina. A computational study of Î±â€Al₂O₃(0001) and Î³â€Al₂O₃(001) using an embeddedâ€cluster approach. Physica Status Solidi (B): Basic Research, 2010, 247, 1023-1031.	0.7	10
128	Structureâ€Dependence of the magnetic moment in small palladium clusters: Surprising results from the M06â€L Metaâ€GGA functional. International Journal of Quantum Chemistry, 2012, 112, 113-120.	1.0	10
129	Thermal Decomposition of Branched Silanes: A Computational Study on Mechanisms. Chemistry - A European Journal, 2012, 18, 9106-9116.	1.7	10
130	Formation of n-hexane from methylcyclopentane via a metallacyclobutane intermediate at step sites of Pt surfaces: Mechanism from first-principles calculations. Journal of Catalysis, 2013, 299, 146-149.	3.1	10
131	Formation of Propane in the Aqueousâ€Phase Processing of 1â€Propanol over Platinum: A DFT Study. ChemCatChem, 2013, 5, 3299-3308.	1.8	10
132	The DFT+Umol method and its application to the adsorption of CO on platinum model clusters. Journal of Chemical Physics, 2014, 140, 174709.	1.2	10
133	Extending the cluster scaling technique to ruthenium clusters with hcp structures. Surface Science, 2016, 643, 156-163.	0.8	10
134	Reactivity trends of the MoVO_xmixed metal oxide catalyst from density functional modeling. Catalysis Science and Technology, 2019, 9, 1559-1569.	2.1	10
135	Load balancing by workâ€“stealing in quantum chemistry calculations: Application to hybrid density functional methods. International Journal of Quantum Chemistry, 2014, 114, 813-822.	1.0	9
136	How the distribution of reduced vanadium centers affects structure and stability of the MoVO_xmaterial. Catalysis Science and Technology, 2018, 8, 2654-2660.	2.1	9
137	DFT Variants for Mixed-Metal Oxides. Benchmarks Using Multi-Center Cluster Models. Journal of Physical Chemistry A, 2018, 122, 7042-7050.	1.1	9
138	Strain and Low-Coordination Effects on Monolayer Nanoislands of Pd and Pt on Au(111): A Comparative Analysis Based on Density Functional Results. Journal of Physical Chemistry C, 2020, 124, 13225-13230.	1.5	9
139	Electronic and Geometric Structure of the Cluster Compound Au₅₅[P(C₆H₅)₃]₁₂C_l6. A Computational Study. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2009, 64, 1246-1258.	0.3	8
140	Small silver clusters at paramagnetic defects of silica surfaces. Surface Science, 2010, 604, 1705-1712.	0.8	8
141	Impurity Atoms on Small Transition Metal Clusters. Insights from Density Functional Model Studies. Topics in Catalysis, 2011, 54, 363-377.	1.3	8
142	Scalable properties of metal clusters: A comparative DFT study of ionic-core treatments. Chemical Physics Letters, 2013, 578, 92-96.	1.2	8
143	Monolayer Nanoislands of Pt on Au and Cu: A First-Principles Computational Study. Journal of Physical Chemistry C, 2014, 118, 22102-22110.	1.5	8
144	Quantum chemical modeling of tri-Mn-substituted W-based Keggin polyoxoanions. Electrochimica Acta, 2017, 231, 659-669.	2.6	8

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145	Ethanol Conversion to Ethylene and Acetaldehyde over Rhodium(I) Exchanged Faujasite Zeolite. A QM/MM and Microkinetic Study. Journal of Physical Chemistry C, 2018, 122, 2783-2795.	1.5	8
146	Câ€“C coupling at a zeolite-supported Rh(<scp>i</scp>) complex. DFT search for the mechanism. Catalysis Science and Technology, 2019, 9, 2781-2793.	2.1	8
147	Theoretical Investigation of the Coordination of N2Ligands to the Cluster Ni3. Journal of Physical Chemistry A, 2004, 108, 6127-6144.	1.1	7
148	Uranyl(VI) Complexation by Sulfonate Ligands: A Relativistic Density Functional and Timeâ€Resolved Laserâ€Induced Fluorescence Spectroscopy Study. European Journal of Inorganic Chemistry, 2012, 2012, 3636-3644.	1.0	7
149	Efficient Two-Step Procedures for Locating Transition States of Surface Reactions. Journal of Chemical Theory and Computation, 2013, 9, 588-599.	2.3	7
150	DFT cluster model study of MoVO-type mixed-metal oxides. Computational and Theoretical Chemistry, 2014, 1045, 57-65.	1.1	7
151	Redox behavior of small metal clusters with respect to hydrogen. The effect of the cluster charge from density functional results. Physical Chemistry Chemical Physics, 2010, 12, 11015.	1.3	6
152	Crystal-Chemical Composition of Dicoctahedral Smectites: An Energy-Based Assessment of Empirical Relations. ACS Earth and Space Chemistry, 2017, 1, 629-636.	1.2	6
153	Relativistic Density Functional Study of the Dinuclear Uranyl Complex [(UO2)2(Î¼2-OH)2Cl2(H2O)4] in Its Crystalline Environment. European Journal of Inorganic Chemistry, 2003, 2003, 3144-3151.	1.0	5
154	Gold-Thiolate Clusters: A Relativistic Density Functional Study of the Model Species Au₁₃(SR)_n, R = H, CH₃, n = 4, 6, 8. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2004, 59, 1585-1599.	0.3	5
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156	Formation of CO₂ and Ethane from Propionyl over Platinum: A Density Functional Theory Study. ACS Catalysis, 2013, 3, 1730-1738.	5.5	5
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