Dennis R Salahub

List of Publications by Year
in descending order

183 papers	18,737 citations	36303 51 h-index	11607 135 g-index
185 all docs	185 docs citations	185 times ranked	13537 citing authors

#	Article	IF	Citations
1	Molecular excitation energies to high-lying bound states from time-dependentâ€‰density-functionalâ€‰responseâ€‰theory: Characterizationâ€‰and correctionâ€‰ofâ€‰theâ€‰time-dependentâ€‰localâ€‰densityâ€‰approximation ionization threshold. Journal of Chemical Physics, 1998, 108, 4439-4449.	3.0	4,596
2	Optimization of Gaussian-type basis sets for local spin density functional calculations. Part I. Boron through neon, optimization technique and validation. Canadian Journal of Chemistry, 1992, 70, 560-571.	1.1	2,791
3	Dynamic polarizabilities and excitation spectra from a molecular implementation of timeâ€dependent densityâ€functional response theory: N2as a case study. Journal of Chemical Physics, 1996, 104, 5134-5147.	3.0	872
4	New algorithm for the optimization of geometries in local density functional theory. Chemical Physics Letters, 1990, 169, 387-392.	2.6	636
5	Density functional theory augmented with an empirical dispersion term. Interaction energies and geometries of 80 noncovalent complexes compared withab initioquantum mechanics calculations. Journal of Computational Chemistry, 2007, 28, 555-569.	3.3	620
6	Nuclear Magnetic Resonance Shielding Tensors Calculated with a Sum-over-States Density Functional Perturbation Theory. Journal of the American Chemical Society, 1994, 116, 5898-5908.	13.7	485
7	Gaussian density functional calculations on hydrogen-bonded systems. Journal of the American Chemical Society, 1992, 114, 4391-4400.	13.7	462
8	Semiempirical Quantum Chemical PM6 Method Augmented by Dispersion and H-Bonding Correction Terms Reliably Describes Various Types of Noncovalent Complexes. Journal of Chemical Theory and Computation, 2009, 5, 1749-1760.	5.3	312
9	Electrical and mechanical properties of distorted carbon nanotubes. Physical Review B, 1999, 60, 13824-13830.	3.2	293
10	Asymptotic correction approach to improving approximate exchangeâ€“correlation potentials: Time-dependent density-functional theory calculations of molecular excitation spectra. Journal of Chemical Physics, 2000, 113, 8918-8935.	3.0	280
11	Assessment of Kohn-Sham density-functional orbitals as approximate Dyson orbitals for the calculation of electron-momentum-spectroscopy scattering cross sections. Physical Review A, 1994, 50, 4707-4728.	2.5	255
12	Charge-transfer correction for improved time-dependent local density approximation excited-state potential energy curves: Analysis within the two-level model with illustration for H2 and LiH. Journal of Chemical Physics, 2000, 113, 7062-7071.	3.0	243
13	Effects of Finite Length on the Electronic Structure of Carbon Nanotubes. Journal of Physical Chemistry B, 1999, 103, 641-646.	2.6	223
14	Structure, bonding, and magnetism of small Fe , Co , and Ni clusters, n â‰¤ 5. Chemical Physics Letters, 1997, 271, 133-142.	2.6	221
15	Density functional study of nitrogen oxides. Journal of Chemical Physics, 1994, 100, 2910-2923.	3.0	196
16	Calculation of spinâ€”spin coupling constants using density functional theory. Chemical Physics Letters, 1994, 221, 91-99.	2.6	192
17	deMon2k. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 548-555.	14.6	189
18	Model potential calculations for secondâ€row transition metal molecules within the localâ€spinâ€density method. Journal of Chemical Physics, 1985, 83, 4573-4580.	3.0	169

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19	Nuclear magnetic resonance spinâ€“spin coupling constants from density functional theory: Problems and results. Journal of Chemical Physics, 1996, 105, 8793-8800.	3.0	146
20	The calculation of NMR and ESR spectroscopy parameters using density functional theory. Theoretical and Computational Chemistry, 1995, 2, 273-347.	0.4	139
21	Spin-orbit correction to NMR shielding constants from density functional theory. Chemical Physics Letters, 1996, 261, 335-345.	2.6	136
22	The structure of Nb3O and Nb3O+ determined by pulsed field ionizationâ€“zero electron kinetic energy photoelectron spectroscopy and density functional theory. Journal of Chemical Physics, 1995, 103, 5335-5342.	3.0	135
23	Density-functional calculations for small iron clusters:Fen,Fen+, andFenâ^'fornâ‰5. Physical Review B, 1994, 49, 11842-11852.	3.2	134
24	Defining the Domain of Density Functionals: Charge-Transfer Complexes. Journal of the American Chemical Society, 1995, 117, 1141-1142.	13.7	133
25	The effect of structural distortions on the electronic structure of carbon nanotubes. Chemical Physics Letters, 1998, 297, 45-50.	2.6	130
26	The hyperfine structures of small radicals from density functional calculations. Journal of Chemical Physics, 1994, 100, 5066-5075.	3.0	126
27	Studying genetic regulatory networks at the molecular level: Delayed reaction stochastic models. Journal of Theoretical Biology, 2007, 246, 725-745.	1.7	121
28	Ground and excited states of group IVA diatomics from localâ€spinâ€density calculations: Model potentials for Si, Ge, and Sn. Journal of Chemical Physics, 1987, 87, 6562-6572.	3.0	120
29	Kohnâ€“Sham orbitals and orbital energies: fictitious constructs but good approximations all the same. Journal of Electron Spectroscopy and Related Phenomena, 2002, 123, 345-363.	1.7	113
30	Zero-Pressure Thermal-Radiation-Induced Dissociation of Gas-Phase Cluster Ions: Comparison of Theory and Experiment for (H2O)2Cl- and (H2O)3Cl-. Journal of the American Chemical Society, 1995, 117, 12819-12825.	13.7	109
31	Multiscale modeling of enzymes: QMâ€cluster, QM/MM, and QM/MM/MD: A tutorial review. International Journal of Quantum Chemistry, 2018, 118, e25558.	2.0	106
32	Topological analysis of the molecular electrostatic potential. Journal of Chemical Physics, 1999, 111, 4893-4905.	3.0	105
33	Gaussian density functional calculations on the allyl and polyene radicals: C3H5 to C11H13. Journal of Chemical Physics, 1991, 95, 4317-4326.	3.0	104
34	Density-functional study of niobium clusters. Physical Review A, 1993, 47, R774-R777.	2.5	104
35	Representation of Ionâ€“Protein Interactions Using the Drude Polarizable Force-Field. Journal of Physical Chemistry B, 2015, 119, 9401-9416.	2.6	101
36	Many-Body Effects in Systems of Peptide Hydrogen-Bonded Networks and Their Contributions to Ligand Binding:Â A Comparison of the Performances of DFT and Polarizable Molecular Mechanics. Journal of Physical Chemistry B, 2000, 104, 9746-9754.	2.6	93

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37	Calculation of ligand NMR chemical shifts in transition-metal complexes using ab initio effective-core potentials and density functional theory. Chemical Physics Letters, 1995, 235, 382-388.	2.6	90
38	Structure and properties of cobalt clusters up to the tetramer: A density-functional study. Physical Review B, 1997, 55, 10905-10921.	3.2	88
39	Using a classical potential as an efficient importance function for sampling from an ab initio potential. Journal of Chemical Physics, 2000, 113, 4852.	3.0	88
40	Scalar Relativistic Effects on 17O NMR Chemical Shifts in Transition-Metal Oxo Complexes. An ab Initio ECP/DFT Study. Journal of the American Chemical Society, 1995, 117, 1851-1852.	13.7	82
41	Density functional calculations of isotropic hyperfine coupling constants of radical cations. Journal of Chemical Physics, 1993, 99, 9756-9763.	3.0	77
42	All-electron local and gradient-corrected density-functional calculations ofNandipole polarizabilities forn=1â€“6. Physical Review B, 1995, 52, 2184-2200.	3.2	77
43	Vibrational and geometric structures of Nb3C2 and Nb3C+2 from pulsed field ionizationâ€zero electron kinetic energy photoelectron spectra and density functional calculations. Journal of Chemical Physics, 1996, 105, 10663-10671.	3.0	71
44	Theoretical study of the structure and binding of iron clusters:Fen(nâ‰5). Physical Review B, 1993, 47, 10955-10958.	3.2	67
45	Cooperative Hydrogen Bonding and Enzyme Catalysis. Angewandte Chemie - International Edition, 1998, 37, 2985-2990.	13.8	66
46	Derivation of interpretative models for long range electron transfer from constrained density functional theory. Computational and Theoretical Chemistry, 2010, 943, 115-120.	1.5	65
47	The accurate calculation of dipole moments and dipole polarizabilities using Gaussian-based density functional methods. International Journal of Quantum Chemistry, 1992, 43, 463-479.	2.0	59
48	A density functional study of FeCO, FeCOâ^', and FeCO+. Journal of Chemical Physics, 1994, 100, 8233-8239.	3.0	59
49	Multilevel Fragment-Based Approach (MFBA): A Novel Hybrid Computational Method for the Study of Large Molecules. Journal of Chemical Theory and Computation, 2010, 6, 91-99.	5.3	58
50	Solvation of formic acid and proton transfer in hydrated clusters. Journal of Chemical Physics, 2002, 116, 6028-6038.	3.0	54
51	V3: Structure and vibrations from density functional theory, Franckâ€“Condon factors, and the pulsed-field ionization zero-electron-kinetic energy spectrum. Journal of Chemical Physics, 2001, 114, 4036-4044.	3.0	53
52	Ab Initio ECP/DFT Calculation and Interpretation of Carbon and Oxygen NMR Chemical Shift Tensors in Transitionâ€Metal Carbonyl Complexes. Chemistry - A European Journal, 1996, 2, 24-30.	3.3	52
53	The effects of nonlocal gradient corrections in density functional calculations of hydrocarbon radical hyperfine structures. International Journal of Quantum Chemistry, 1994, 52, 879-901.	2.0	51
54	Site segregation in small rhodium bimetallic aggregates: a combined catalytic and quantum chemical study. Journal of the American Chemical Society, 1991, 113, 1485-1492.	13.7	50

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55	Surface residues dynamically organize water bridges to enhance electron transfer between proteins. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 11799-11804.	7.1	50
56	Influence of Intermolecular Interactions on the 13C NMR Shielding Tensor in Solid .alpha.-Glycine. Journal of the American Chemical Society, 1995, 117, 3294-3295.	13.7	49
57	Scattered-wave calculations of photoionization cross-sections and asymmetry parameters for CO, H2O and H2S. Journal of Electron Spectroscopy and Related Phenomena, 1980, 19, 273-284.	1.7	46
58	Exchange-only optimized effective potential for molecules from resolution-of-the-identity techniques: Comparison with the local density approximation, with and without asymptotic correction. Journal of Chemical Physics, 2002, 116, 8276.	3.0	46
59	Density functional study of mononitrosyls of first-row transition-metal atoms. Journal of Chemical Physics, 1997, 106, 8778-8787.	3.0	45
60	Simple but efficient correlation functional from a model pair-correlation function. Physical Review B, 1994, 49, 7874-7886.	3.2	43
61	Molecular orbital study of structural changes on oxidation and reduction of S3, S4, S6, and S8. Journal of the American Chemical Society, 1978, 100, 7847-7859.	13.7	42
62	Calculation of equilibrium geometries and harmonic frequencies by theLCGTO-MCP-local spin density method. International Journal of Quantum Chemistry, 1990, 38, 29-39.	2.0	42
63	Quantum Effects in Cation Interactions with First and Second Coordination Shell Ligands in Metalloproteins. Journal of Chemical Theory and Computation, 2015, 11, 4992-5001.	5.3	42
64	Chemisorption and diffusion of atomic hydrogen in and on cluster models of palladium, rhodium and bimetallic palladium tin, rhodium tin, and rhodium zinc catalysts. Journal of the American Chemical Society, 1990, 112, 8239-8247.	13.7	41
65	Critical Role of Anisotropy for the Dimerization Energies of Two Proteinâ^'Protein Recognition Motifs:cis-N-Methylacetamide versus a Î²-Sheet Conformer of Alanine Dipeptide. A Joint ab Initio, Density Functional Theory, and Molecular Mechanics Investigation. Journal of the American Chemical Society, 1999, 121, 7885-7894.	13.7	41
66	Characterization of the active site of yeast RNA polymerase II by DFT and ReaxFF calculations. Theoretical Chemistry Accounts, 2008, 120, 479-489.	1.4	41
67	Simulating Electron Dynamics in Polarizable Environments. Journal of Chemical Theory and Computation, 2017, 13, 3985-4002.	5.3	41
68	Model potential for As and LCGTO MP LSD calculation of geometry, electronic structure and photoelectron spectra for As2 and As4. Chemical Physics Letters, 1987, 142, 169-174.	2.6	40
69	Aluminum clusters. A comparison between all electron and model core potential calculations. Journal of Chemical Physics, 1994, 101, 10677-10685.	3.0	39
70	Assessment of the quality of orbital energies in resolution-of-the-identity Hartreeâ€“Fock calculations using deMon auxiliary basis sets. Journal of Chemical Physics, 2001, 114, 7342-7350.	3.0	38
71	Lead-free, stable mixed halide double perovskites Cs2AgBiBr6 and Cs2AgBiBr6â^'xClx â€“ A detailed theoretical and experimental study. Chemical Physics, 2020, 529, 110547.	1.9	38
72	Analysis and assignment of the optical absorption transitions in CuCl2 with Gaussian density functional calculations. Chemical Physics Letters, 1994, 219, 228-236.	2.6	37

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73	Intramolecular interaction energies in model alanine and glycine tetrapeptides. Evaluation of anisotropy, polarization, and correlation effects. A parallelab initioHF/MP2, DFT, and polarizable molecular mechanics study. Journal of Computational Chemistry, 2004, 25, 823-834.	3.3	37
74	Density functional theory and quantum chemistry: Metals and metal oxides. Journal of Molecular Catalysis, 1993, 82, 117-129.	1.2	35
75	The backbone 15N chemical shift tensor of the gramicidin channel. A molecular dynamics and density functional study. Chemical Physics Letters, 1995, 239, 186-194.	2.6	31
76	Quantum effects in biological electron transfer. Physical Chemistry Chemical Physics, 2012, 14, 5902.	2.8	31
77	Selective ion binding and transport by membrane proteins â€“ A computational perspective. Coordination Chemistry Reviews, 2017, 345, 108-136.	18.8	31
78	Band theory for the magnetic moment in the bcc Fe-Co alloy. Physical Review B, 1982, 25, 3427-3429.	3.2	30
79	Molecular and electronic structure of ozone and thiozone from LCAO local density calculations. Canadian Journal of Chemistry, 1985, 63, 1982-1987.	1.1	29
80	Embedded cluster model for chemisorption using density functional calculations: Oxygen adsorption on the Al(100) surface.. Journal of Chemical Physics, 1998, 108, 743-756.	3.0	29
81	Fe(N2)n(n= 1â^'5):Â Structure, Bonding, and Vibrations from Density Functional Theory. Inorganic Chemistry, 1999, 38, 3895-3903.	4.0	29
82	QM/MM calculations of EPR hyperfine coupling constants in blue copper proteins. Computational and Theoretical Chemistry, 2003, 632, 287-295.	1.5	29
83	First-principles calculations of the structural, mechanical, electronic and bonding properties of (CrB) Tj ETQq1 1 0.784314 rgBT /Overlo	5.5	29
84	Molecular Simulations with in-deMon2k QM/MM, a Tutorial-Review. Molecules, 2019, 24, 1653.	3.8	29
85	Molybdenum Carbide Nanocatalysts at Work in the in Situ Environment: A Density Functional Tight-Binding and Quantum Mechanical/Molecular Mechanical Study. Journal of the American Chemical Society, 2015, 137, 4249-4259.	13.7	28
86	Radical pairs may play a role in xenon-induced general anesthesia. Scientific Reports, 2021, 11, 6287.	3.3	28
87	Kohnâ€“Sham density-functional study of the formation of benzene from acetylene on iron clusters, Fe/Fen+â€‰(n=1â€“4). Journal of Chemical Physics, 2003, 119, 12291-12300.	3.0	27
88	A Guide to QM/MM Methodology and Applications. Advances in Quantum Chemistry, 2010, 59, 353-400.	0.8	27
89	The structure of triniobium dinitride from zero electron kinetic energy photoelectron spectroscopy and density functional calculations. Chemical Physics Letters, 1997, 277, 71-78.	2.6	26
90	Effect of rotation and vibration on nuclear magnetic resonance chemical shifts: Density functional theory calculations. Journal of Chemical Physics, 1999, 110, 7153-7159.	3.0	26

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91	Adsorption of Hexacyclic C₆H₆, C₆H₈, C₆H₁₀, and C₆H₁₂ on a Mo-Terminated Î±-Mo₂C (0001) Surface. Journal of Physical Chemistry C, 2013, 117, 7069-7080.	3.1	26
92	LCGTO MP LSD calculations for the diatomics PdX (X = C, Si, Ge, Sn). Chemical Physics, 1987, 114, 331-338.	1.9	25
93	A density functional study of the interaction of CO2 with a Pd atom. International Journal of Quantum Chemistry, 1994, 52, 645-654.	2.0	25
94	LiCl solvation in N-methyl-acetamide (NMA) as a model for understanding Li⁺binding to an amide plane. Physical Chemistry Chemical Physics, 2016, 18, 4191-4200.	2.8	23
95	Reaction of a Mo Atom with H2, N2, and O2:â€‰ A Density Functional Study. Journal of Physical Chemistry A, 1997, 101, 1532-1541.	2.5	22
96	Transmission Coefficients for Chemical Reactions with Multiple States: Role of Quantum Decoherence. Journal of the American Chemical Society, 2011, 133, 3883-3894.	13.7	22
97	Scalar Relativistic Effects on 17O NMR Chemical Shifts in Transition-Metal Oxo Complexes. An ab Initio ECP/DFT Study. [Erratum to document cited in CA122:254385]. Journal of the American Chemical Society, 1995, 117, 8492-8492.	13.7	21
98	The QMâ€MM interface for CHARMMâ€deMon. Journal of Computational Chemistry, 2010, 31, 1015-1023.	3.3	21
99	Core-level shifts from density-functional computations. Physical Review B, 1993, 47, 12992-12994.	3.2	20
100	Time-dependent density functional theory as a foundation for a firmer understanding of sum-over-states density functional perturbation theory: ?Loc.3? approximation. International Journal of Quantum Chemistry, 2003, 91, 67-83.	2.0	20
101	Native Defects in Î±-Mo₂C: Insights from First-Principles Calculations. Journal of Physical Chemistry C, 2014, 118, 25517-25524.	3.1	20
102	QM/MM Calculations with deMon2k. Molecules, 2015, 20, 4780-4812.	3.8	20
103	On the electronic structure of MoO: Spin-polarized density functional calculations of spectroscopic properties of low-lying quintet, triplet, and septet states. International Journal of Quantum Chemistry, 1994, 52, 1017-1026.	2.0	19
104	Negative ion photoelectron spectra simulation of V3O from a density functional study. Journal of Chemical Physics, 2003, 118, 4913-4919.	3.0	19
105	An efficient Monte Carlo method for calculating ab initio transition state theory reaction rates in solution. Journal of Chemical Physics, 2003, 119, 11285-11297.	3.0	19
106	Reparameterization of a meta-generalized gradient approximation functional by combining TPSS exchange with Ï„1 correlation. Theoretical Chemistry Accounts, 2007, 118, 693-707.	1.4	19
107	Lipid Thermodynamics: Melting is Molecular. ChemPhysChem, 2008, 9, 2321-2324.	2.1	19
108	Progress and challenges in simulating and understanding electron transfer in proteins. Archives of Biochemistry and Biophysics, 2015, 582, 28-41.	3.0	19

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109	Delay stochastic simulation of singleâ€gene expression reveals a detailed relationship between protein noise and mean abundance. FEBS Letters, 2008, 582, 2905-2910.	2.8	18
110	Radical pairs may explain reactive oxygen species-mediated effects of hypomagnetic field on neurogenesis. PLoS Computational Biology, 2022, 18, e1010198.	3.2	18
111	NO adsorption on Pd clusters. A density functional study. Topics in Catalysis, 1999, 9, 123-133.	2.8	17
112	Kohnâ€“Sham density-functional study of the adsorption of acetylene and vinylidene on iron clusters, Fen/Fen+ (n=1â€“4). Journal of Chemical Physics, 2003, 119, 12279-12290.	3.0	17
113	NO/Ni, NO/Ni2, and (NO)2/Ni2Interactions. A Density Functional Study. Journal of Physical Chemistry B, 1997, 101, 7464-7471.	2.6	16
114	Origin of the high basicity of 2,7-dimethoxy-1,8-bis(dimethylamino)naphthalene: implications for enzyme catalysis. Computational and Theoretical Chemistry, 2001, 547, 113-118.	1.5	16
115	Density functional study of benzene adsorption on the Î±-Mo2C(0001) surface. Structural Chemistry, 2012, 23, 1459-1466.	2.0	16
116	Density functional study on the reaction of CO molecules with MgO surfaces. Catalysis Today, 1995, 23, 357-364.	4.4	15
117	A density functional study of borane and alane monoammoniate (BH3NH3,AlH3NH3). Journal of Chemical Physics, 1995, 103, 7408-7413.	3.0	15
118	Investigation of Mï¿½ssbauer parameters for a set of iodine compounds using gradient-corrected density functional theory. International Journal of Quantum Chemistry, 1997, 63, 575-583.	2.0	15
119	14,15N NMR Shielding Constants from Density Functional Theory. Journal of Physical Chemistry A, 2003, 107, 9924-9930.	2.5	15
120	Asymptotic Expansion for Electrostatic Embedding Integrals in QM/MM Calculations. Journal of Chemical Theory and Computation, 2012, 8, 4232-4238.	5.3	15
121	Reliability of semiempirical and DFTB methods for the global optimization of the structures of nanoclusters. Journal of Molecular Modeling, 2020, 26, 303.	1.8	15
122	Molecular versus Dissociative Chemisorption of Nitric Oxide on Co2and Co3(Neutral and Cationic). A Density Functional Study. Journal of Physical Chemistry A, 1998, 102, 4643-4651.	2.5	14
123	Spinâ€driven activation of dioxygen in various metalloenzymes and their inspired models. Journal of Computational Chemistry, 2011, 32, 1178-1182.	3.3	14
124	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>A</mml:mi><mml:mi>b</mml:mi></mml:mrow><mml:mo and group theoretical study of properties of a carbon trimer defect in hexagonal boron nitride. Physical Review B, 2022, 105, .	3.2	13
125	Electron deformation density distribution for cyclic octasulfur by the SCF-X.alpha.-SW method. Journal of the American Chemical Society, 1977, 99, 8067-8068.	13.7	12
126	Explanation for the structural differences of S2+4, S04 and S2â¯4. Chemical Physics Letters, 1978, 57, 33-36.	2.6	12

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127	Quintet electronic states of MoO: Gaussian density functional calculations. International Journal of Quantum Chemistry, 1992, 44, 393-399.	2.0	12
128	A new active learning approach for global optimization of atomic clusters. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	12
129	Geometrical, spectroscopic, and magnetic properties of an oxygen atom adsorbed on the Ni(100) surface. International Journal of Quantum Chemistry, 1993, 48, 277-286.	2.0	11
130	Bonding in Nb[sub 3]O, Nb[sub 3]S and Nb[sub 3]Se: A topological analysis of the electrostatic potential. Journal of Chemical Physics, 2001, 114, 819.	3.0	11
131	Dissociation, solvation, and dynamics of HBr in small water clusters. Theoretical Chemistry Accounts, 2005, 114, 115-123.	1.4	11
132	Dioxygen Activation by Mononuclear Copper Enzymes: Insights from a Tripodal Ligand Mimicking Their CuM Coordination Sphere. Inorganic Chemistry, 2009, 48, 7003-7005.	4.0	11
133	Editorial: Special issue on quantum mechanical modeling of biological systems. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 1-2.	3.6	11
134	The role of metal substitution in the promiscuity of natural and artificial carbonic anhydrases. Coordination Chemistry Reviews, 2017, 345, 73-85.	18.8	11
135	Explicit Water Molecules Play a Key Role in the Mechanism of Rhodiumâ€Substituted Human Carbonic Anhydrase. ChemCatChem, 2017, 9, 1047-1053.	3.7	11
136	Retardation in electron dynamics simulations based on time-dependent density functional theory. European Physical Journal D, 2018, 72, 1.	1.3	11
137	NMR shieldings from sum-over-states density-functional-perturbation theory: Further testing of the â€œLoc.3â€•approximation. Journal of Chemical Physics, 2003, 118, 6758-6768.	3.0	10
138	Quantum Chemical Molecular Dynamics Study of the Waterâ€“Gas Shift Reaction on a Pd/MgO(100) Catalyst Surface. Journal of Physical Chemistry C, 2013, 117, 5051-5066.	3.1	10
139	Heterogeneous reactions of SO2 on the hematite(0001) surface. Journal of Chemical Physics, 2018, 149, 194703.	3.0	10
140	Taking the multiplicity inside the loop: active learning for structural and spin multiplicity elucidation of atomic clusters. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	10
141	Multiscale molecular modelling: from electronic structure to dynamics of nanosystems and beyond. Physical Chemistry Chemical Physics, 2022, 24, 9051-9081.	2.8	10
142	Charge distributions and chemical effects. XVIII. On the relationship between total valenceâ€electron energies and nuclearâ€“electronic interaction energies in atoms and ions. Journal of Chemical Physics, 1978, 69, 3321-3324.	3.0	9
143	Spin-orbit coupling in the local spin density-scattered wave method. Chemical Physics Letters, 1989, 159, 472-478.	2.6	9
144	Bis(phosphine)nickelacyclopentane: an investigation by local spin density theory. Inorganic Chemistry, 1990, 29, 1544-1549.	4.0	9

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145	Bond selectivity in the dissociative adsorption of c-CH2N2 on single crystals: a comparative DFT-LSD investigation for Pd(110) and Cu(110). Surface Science, 1996, 347, 11-24.	1.9	9
146	Recent Progress in Density Functional Methodology for Biomolecular Modeling. Structure and Bonding, 2013, , 1-64.	1.0	9
147	Benchmarking polarizable and non-polarizable force fields for Ca2+â€“peptides against a comprehensive QM dataset. Journal of Chemical Physics, 2020, 153, 144102.	3.0	9
148	Electrostatic fields E(r) created in the vicinity of cluster-modelled nickel surfaces, using DFT densities. Computational and Theoretical Chemistry, 1995, 330, 279-285.	1.5	8
149	Achieving reliability of calculations for flat potential surfaces in density functional theory: The case of Al4 and Al4+1. International Journal of Quantum Chemistry, 1997, 63, 301-311.	2.0	8
150	Chemical nature of point defects at the (VO) 2 P 2 O 7 (100) surface. Surface Science, 2003, 538, 160-170.	1.9	8
151	Structural analysis of phosphatidyl choline lipids and glycerol precursors. Canadian Journal of Chemistry, 2009, 87, 1261-1267.	1.1	8
152	Electron density in Si2and Cl2. Molecular Physics, 1980, 41, 509-517.	1.7	7
153	Interaction of atomic hydrogen with cluster models of Pd, Rh and bimetallic PdSn and RhSn catalysts. Surface Science, 1990, 235, L319-L323.	1.9	7
154	Applications of the adiabatic connection method to conformational equilibria and reactions involving formic acid. Computers & Chemistry, 1995, 19, 145-154.	1.2	7
155	Temperature dependence of the molecular conformations of dilauroyl phosphatidylcholine: A density functional study. International Journal of Quantum Chemistry, 2013, 113, 631-636.	2.0	7
156	Comment on â€˜â€˜Density functional calculation of nuclear magnetic resonance chemical shiftsâ€™â€™ [J. Chem. Phys. 102, 2806 (1995)]. Journal of Chemical Physics, 1996, 104, 1163-1164.	3.0	6
157	A reparametrization of a meta-GGA exchange-correlation functional with improved descriptions of van der Waals interactions. Chemical Physics Letters, 2007, 436, 394-399.	2.6	6
158	Nelfinavir: A magic bullet to annihilate cancer cells. Cancer Biology and Therapy, 2009, 8, 233-235.	3.4	6
159	A theoretical study of the mechanism of the nucleotidyl transfer reaction catalyzed by yeast RNA polymerase II. Science China Chemistry, 2012, 55, 1887-1894.	8.2	6
160	Auxiliary Density Functional Theory: From Molecules to Nanostructures. , 2017, , 795-860.		6
161	Electronic properties of carbon nanotubes complexed with a DNA nucleotide. Physical Chemistry Chemical Physics, 2017, 19, 7333-7342.	2.8	6
162	Self-Consistent Auxiliary Density Perturbation Theory. Journal of Chemical Theory and Computation, 2021, 17, 6934-6946.	5.3	6

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163	A new active learning approach for adsorbateâ€“substrate structural elucidation in silico. Journal of Molecular Modeling, 2022, 28, .	1.8	6
164	XSnS₃ (X = Ga, In) monolayer semiconductors as photo-catalysts for water splitting: a first principles study. Journal of Materials Chemistry C, 2022, 10, 11412-11423.	5.5	6
165	Computational investigation of Ba2ZrTiO6 double perovskite for optoelectronic and thermoelectric applications. Journal of Solid State Chemistry, 2022, 314, 123385.	2.9	6
166	Auxiliary Density Functional Theory: From Molecules to Nanostructures. , 2015, , 1-67.		5
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