Johannes Neugebauer

List of Publications by Year
in descending order

150	6,472	50170	74018
papers	citations	46 h-index	75 g-index

164	164	164	4210
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Solvation Free Energies in Subsystem Density Functional Theory. Journal of Chemical Theory and Computation, 2022, 18, 723-740.	2.3	12
2	The Seamless Connection of Local and Collective Excited States in Subsystem Time-Dependent Density Functional Theory. Journal of Physical Chemistry Letters, 2022, 13, 1003-1018.	2.1	13
3	Origin invariant electronic circular dichroism in the length dipole gauge without London atomic orbitals. Journal of Chemical Physics, 2022, 156, 154114.	1.2	7
4	Automated Generation of Optimized Auxiliary Basis Sets for Long-Range-Corrected TDDFT Using the Cholesky Decomposition. Journal of Chemical Theory and Computation, 2022, 18, 2959-2974.	2.3	5
5	Azo bond formation on metal surfaces. Angewandte Chemie - International Edition, 2021, 60, 1458-1464.	7.2	6
6	Azobindungsbildung auf MetalloberflÃchen. Angewandte Chemie, 2021, 133, 1478-1485.	1.6	0
7	Electronic effects in profluorescent benzotriazinyl radicals: a combined experimental and theoretical study. Physical Chemistry Chemical Physics, 2021, 23, 2999-3007.	1.3	3
8	Synthesis of Ruthenium(II) Complexes Bearing Macrocyclic [11]ane-P₂C^{NHC} Ligands by a Template-Controlled Domino Reaction. Organometallics, 2021, 40, 606-617.	1.1	4
9	Pragmatic Improvement of Magnetic Exchange Couplings from Subsystem Density-Functional Theory through Orthogonalization of Subsystem Orbitals. Journal of Physical Chemistry C, 2021, 125, 6176-6188.	1.5	3
10	Subsystem-Based GW/Betheâ€“Salpeter Equation. Journal of Chemical Theory and Computation, 2021, 17, 2186-2199.	2.3	12
11	Polymerization of silanes through dehydrogenative Siâ€“Si bond formation on metal surfaces. Nature Chemistry, 2021, 13, 350-357.	6.6	11
12	Theoretical Assessment of Hinge-Type Models for Electron Donors in Reaction Centers of Photosystems I and II as well as of Purple Bacteria. Journal of Physical Chemistry B, 2021, 125, 3066-3079.	1.2	6
13	Protein Response Effects on Cofactor Excitation Energies from First Principles: Augmenting Subsystem Time-Dependent Density-Functional Theory with Many-Body Expansion Techniques. Journal of Chemical Theory and Computation, 2021, 17, 6105-6121.	2.3	9
14	Multi-state formulation of the frozen-density embedding quasi-diabatization approach. Journal of Chemical Physics, 2021, 155, 174104.	1.2	4
15	Direct orbital selection within the domain-based local pair natural orbital coupled-cluster method. Journal of Chemical Physics, 2021, 155, 224102.	1.2	9
16	Subsystem density-functional theory for interacting open-shell systems: spin densities and magnetic exchange couplings. Faraday Discussions, 2020, 224, 201-226.	1.6	8
17	Density functional theory based embedding approaches for transition-metal complexes. Physical Chemistry Chemical Physics, 2020, 22, 26093-26103.	1.3	12
18	Electronic couplings for photo-induced processes from subsystem time-dependent density-functional theory: The role of the diabatization. Journal of Chemical Physics, 2020, 153, 184113.	1.2	12

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19	Aryl Triflates in Onâ€Surface Chemistry. Chemistry - A European Journal, 2020, 26, 16727-16732.	1.7	1
20	Orbital Alignment for Accurate Projection-Based Embedding Calculations along Reaction Paths. Journal of Chemical Theory and Computation, 2020, 16, 3607-3619.	2.3	11
21	Design of Ru(II)-NHC-Diamine Precatalysts Directed by Ligand Cooperation: Applications and Mechanistic Investigations for Asymmetric Hydrogenation. Journal of the American Chemical Society, 2020, 142, 7100-7107.	6.6	53
22	Analysis of environment response effects on excitation energies within subsystemâ€based timeâ€dependent densityâ€functional theory. International Journal of Quantum Chemistry, 2020, 120, e26213.	1.0	22
23	Approximate versus Exact Embedding for Chiroptical Properties: Reconsidering Failures in Potential and Response. Journal of Chemical Theory and Computation, 2020, 16, 3104-3120.	2.3	18
24	Computational Investigation of the Spin-Density Asymmetry in Photosynthetic Reaction Center Models from First Principles. Journal of Physical Chemistry B, 2020, 124, 4873-4888.	1.2	13
25	Analysis of the electronic structure of the primary electron donor of photosystemÂI of <i>Spirodela</i> <i>oligorrhiza</i> by photochemically induced dynamic nuclear polarization (photo-CIDNP) solid-state nuclear magnetic resonance (NMR). Magnetic Resonance, 2020, 1, 261-274.	0.8	6
26	Automatic basis-set adaptation in projection-based embedding. Journal of Chemical Physics, 2019, 150, 184104.	1.2	29
27	Regioselective N- and C-Metalation of Neutral 2-Halogenobenzimidazole Derivatives. Organometallics, 2019, 38, 3278-3285.	1.1	10
28	Metal Hydride Vibrations: The Trans Effect of the Hydride. Inorganic Chemistry, 2019, 58, 12467-12479.	1.9	10
29	Intermolecular coupling and intramolecular cyclization of aryl nitriles on Au(111). Chemical Communications, 2019, 55, 11611-11614.	2.2	6
30	Direct orbital selection for projection-based embedding. Journal of Chemical Physics, 2019, 150, 214106.	1.2	18
31	Exact subsystem time-dependent density-functional theory. Journal of Chemical Physics, 2019, 150, 181101.	1.2	30
32	15N photo-CIDNP MAS NMR analysis of a bacterial photosynthetic reaction center of Rhodobacter sphaeroides wildtype. Journal of Chemical Physics, 2019, 151, 195101.	1.2	8
33	Inter-subsystem charge-transfer excitations in exact subsystem time-dependent density-functional theory. Journal of Chemical Physics, 2019, 151, 174109.	1.2	25
34	Optimizing bidentate N-heterocyclic carbene ligands for the modification of late transition metal surfaces â€“ new insights through theory. Physical Chemistry Chemical Physics, 2019, 21, 24926-24934.	1.3	3
35	Towards reliable references for electron paramagnetic resonance parameters based on quantum chemistry: the case of verdazyl radicals. Physical Chemistry Chemical Physics, 2018, 20, 7661-7675.	1.3	8
36	Î±-Diazo Ketones in On-Surface Chemistry. Journal of the American Chemical Society, 2018, 140, 6000-6005.	6.6	24

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37	DFT methods applied to answer the question: how accurate is the ligand acidity constant method for estimating the pK_a of transition metal hydride complexes MHXL₄ when X is varied?. Dalton Transactions, 2018, 47, 2739-2747.	1.6	11
38	S<scp>erenity</scp>: A subsystem quantum chemistry program. Journal of Computational Chemistry, 2018, 39, 788-798.	1.5	57
39	Embedding Methods in Quantum Chemistry. , 2018, , 139-179.		20
40	Antiferromagnetic ordering based on intermolecular London dispersion interactions in amphiphilic TEMPO ammonium salts. Physical Chemistry Chemical Physics, 2018, 20, 28979-28983.	1.3	5
41	Photochemically induced dynamic nuclear polarization NMR on photosystem II: donor cofactor observed in entire plant. Scientific Reports, 2018, 8, 17853.	1.6	16
42	Geometry Optimizations in a Subsystem Density Functional Theory Formalism: A Benchmark Study. Journal of Chemical Theory and Computation, 2018, 14, 5631-5644.	2.3	9
43	Accurate embedding through potential reconstruction: A comparison of different strategies. Journal of Chemical Physics, 2018, 149, 054103.	1.2	19
44	Frozen-density embedding as a quasi-diabatization tool: Charge-localized states for spin-density calculations. Journal of Chemical Physics, 2018, 148, 214104.	1.2	13
45	Reaction Selectivity in Onâ€Surface Chemistry by Surface Coverage Controlâ€”Alkyne Dimerization versus Alkyne Trimerization. Chemistry - A European Journal, 2018, 24, 15303-15308.	1.7	9
46	Ferro- or antiferromagnetism? Heisenberg chains in the crystal structures of verdazyl radicals. Physical Chemistry Chemical Physics, 2018, 20, 22902-22908.	1.3	7
47	Excitation energies of embedded open-shell systems: Unrestricted frozen-density-embedding time-dependent density-functional theory. Journal of Chemical Physics, 2018, 149, 074102.	1.2	12
48	Including protein density relaxation effects in first-principles embedding calculations of cofactor excitation energies. Molecular Physics, 2017, 115, 526-537.	0.8	9
49	Synthesis and Reactivity of Intramolecularly NHC-Stabilized Germylenes and Stannylenes. Organometallics, 2017, 36, 1001-1008.	1.1	15
50	Formation of Organometallic Intermediate States in Onâ€Surface Ullmann Couplings. Chemistry - A European Journal, 2017, 23, 6190-6197.	1.7	36
51	Intermolecular On-Surface Ïƒ-Bond Metathesis. Journal of the American Chemical Society, 2017, 139, 7012-7019.	6.6	40
52	Quantum Chemical Spin Densities for Radical Cations of Photosynthetic Pigment Models. Photochemistry and Photobiology, 2017, 93, 815-833.	1.3	9
53	Cooperative Magnetism in Crystalline Nâ€Arylâ€Substituted Verdazyl Radicals: Firstâ€Principles Predictions and Experimental Results. Chemistry - A European Journal, 2017, 23, 6069-6082.	1.7	12
54	Analytical gradients for subsystem density functional theory within the slaterâ€functionâ€based amsterdam density functional program. Journal of Computational Chemistry, 2017, 38, 238-249.	1.5	10

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55	OberflÃchenâ€Dominoreaktion: Glaserâ€Kupplung und dehydrierende Kupplung von DicarbonsÃuren unter Bildung eines polymeren Bisacylperoxids. Angewandte Chemie, 2016, 128, 9929-9934.	1.6	7
56	Radical perfluoroalkylation â€“ easy access to 2-perfluoroalkylindol-3-imines via electron catalysis. Chemical Communications, 2016, 52, 5997-6000.	2.2	45
57	Benchmarking Electron Densities and Electrostatic Potentials of Proteins from the Three-Partition Frozen Density Embedding Method. Journal of Chemical Theory and Computation, 2016, 12, 4843-4855.	2.3	11
58	Black-box determination of temperature-dependent susceptibilities for crystalline organic radicals with complex magnetic topologies. Physical Chemistry Chemical Physics, 2016, 18, 28262-28273.	1.3	10
59	A Cyclometalated Ruthenium-NHC Precatalyst for the Asymmetric Hydrogenation of (Hetero)arenes and Its Activation Pathway. Organometallics, 2016, 35, 3641-3646.	1.1	42
60	NHC-Catalyzed Enantioselective Dearomatizing Hydroacylation of Benzofurans and Benzothiophenes for the Synthesis of Spirocycles. ACS Catalysis, 2016, 6, 5735-5739.	5.5	70
61	Onâ€Surface Domino Reactions: Glaser Coupling and Dehydrogenative Coupling of a Biscarboxylic Acid To Form Polymeric Bisacylperoxides. Angewandte Chemie - International Edition, 2016, 55, 9777-9782.	7.2	50
62	Editorial for PCCP themed issue â€œDevelopments in Density Functional Theoryâ€• Physical Chemistry Chemical Physics, 2016, 18, 20864-20867.	1.3	0
63	Analytical gradients for excitation energies from frozen-density embedding. Physical Chemistry Chemical Physics, 2016, 18, 20955-20975.	1.3	15
64	Enantiospecific formation of a metal-mediated base pair inside a DNA duplex. Inorganica Chimica Acta, 2016, 452, 181-187.	1.2	28
65	No need for external orthogonality in subsystem density-functional theory. Physical Chemistry Chemical Physics, 2016, 18, 21001-21009.	1.3	21
66	Excitation energies from frozen-density embedding with accurate embedding potentials. Journal of Chemical Physics, 2015, 142, 234101.	1.2	23
67	Sequential Surface Modification of Au Nanoparticles: From Surfaceâ€Bound Ag^I Complexes to Ag⁰ Doping. Chemistry - A European Journal, 2015, 21, 4541-4545.	1.7	5
68	Dioxygen Activation by an in situ Reduced Cu^{II} Hydrazone Complex. European Journal of Inorganic Chemistry, 2015, 2015, 4006-4012.	1.0	6
69	Subsystem-DFT potential-energy curves for weakly interacting systems. Physical Chemistry Chemical Physics, 2015, 17, 14323-14341.	1.3	33
70	Part and whole in wavefunction/DFT embedding. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	30
71	Regioselectivity of the C-Metalation of 6-Furylpurine: Importance of Directing Effects. Inorganic Chemistry, 2015, 54, 4183-4185.	1.9	9
72	Self-consistent embedding of density-matrix renormalization group wavefunctions in a density functional environment. Journal of Chemical Physics, 2015, 142, 044111.	1.2	34

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73	A Local Variant of the Conductor-Like Screening Model for Fragment-Based Electronic-Structure Methods. Journal of Chemical Theory and Computation, 2015, 11, 5277-5290.	2.3	14
74	Describing long-range charge-separation processes with subsystem density-functional theory. Journal of Chemical Physics, 2014, 140, 164103.	1.2	39
75	Wavefunction in Density Functional Theory Embedding for Excited States: Which Wavefunctions, which Densities?. ChemPhysChem, 2014, 15, 3205-3217.	1.0	60
76	Calculation of Complex Bio- and Organic Systems: From Ground-State Reactivity and Spectroscopy to Excited-State Dynamics. ChemPhysChem, 2014, 15, 3139-3140.	1.0	3
77	Subsystem densityâ€functional theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 325-362.	6.2	282
78	Vibronic-structure tracking: A shortcut for vibrationally resolved UV/Vis-spectra calculations. Journal of Chemical Physics, 2014, 141, 164115.	1.2	13
79	Decarboxylative Polymerization of 2,6-Naphthalenedicarboxylic Acid at Surfaces. Journal of the American Chemical Society, 2014, 136, 9658-9663.	6.6	114
80	Modeling environment effects on pigment site energies: Frozen density embedding with fully quantum-chemical protein densities. Computational and Theoretical Chemistry, 2014, 1040-1041, 347-359.	1.1	21
81	Protein Effects on the Optical Spectrum of the Fennaâ€“Matthewsâ€“Olson Complex from Fully Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2013, 9, 1808-1820.	2.3	58
82	Exciton Coupling Mechanisms Analyzed with Subsystem TDDFT: Direct vs Pseudo Exchange Effects. Journal of Physical Chemistry B, 2013, 117, 3480-3487.	1.2	17
83	State-Specific Embedding Potentials for Excitation-Energy Calculations. Journal of Chemical Theory and Computation, 2013, 9, 2355-2367.	2.3	70
84	Direct determination of exciton couplings from subsystem time-dependent density-functional theory within the Tammâ€“Dancoff approximation. Journal of Chemical Physics, 2013, 138, 034104.	1.2	41
85	An accurate and linear-scaling method for calculating charge-transfer excitation energies and diabatic couplings. Journal of Chemical Physics, 2013, 138, 054101.	1.2	67
86	Orbital-Free Embedding Calculations of Electronic Spectra. Recent Advances in Computational, 2013, , 323-354.	0.8	6
87	Spin densities from subsystem density-functional theory: Assessment and application to a photosynthetic reaction center complex model. Journal of Chemical Physics, 2012, 136, 194104.	1.2	35
88	Selective TDDFT with automatic removal of ghost transitions: application to a perylene-dye-sensitized solar cell model. Physical Chemistry Chemical Physics, 2012, 14, 8608.	1.3	13
89	M<scp>O</scp>V<scp>I</scp>P<scp>AC</scp>: Vibrational spectroscopy with a robust metaâ€program for massively parallel standard and inverse calculations. Journal of Computational Chemistry, 2012, 33, 2186-2198.	1.5	59
90	Mechanism and Reaction Coordinate of Directional Charge Separation in Bacterial Reaction Centers. Journal of Physical Chemistry Letters, 2012, 3, 694-697.	2.1	42

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91	Quantum Chemical Description of Absorption Properties and Excitedâ€State Processes in Photosynthetic Systems. ChemPhysChem, 2012, 13, 386-425.	1.0	107
92	First-principles calculation of electronic spectra of light-harvesting complex II. Physical Chemistry Chemical Physics, 2011, 13, 10475.	1.3	67
93	Theoretical Spectroscopy of Astaxanthin in Crustacyanin Proteins: Absorption, Circular Dichroism, and Nuclear Magnetic Resonance. Journal of Physical Chemistry B, 2011, 115, 3216-3225.	1.2	33
94	Response to â€œComment on â€˜Accurate frozen-density embedding potentials as a first step towards a subsystem description of covalent bondsâ€™â€•[J. Chem. Phys. 135, 027101 (2011)]. Journal of Chemical Physics, 2011, 135, 027102.	1.2	9
95	Potential-energy surfaces of local excited states from subsystem- and selective Kohnâ€“Sham-TDDFT. Chemical Physics, 2011, 391, 147-156.	0.9	15
96	Modelling charge transfer reactions with the frozen density embedding formalism. Journal of Chemical Physics, 2011, 135, 234103.	1.2	87
97	The Resonance Raman Spectra of Spheroidene Revisited with a Firstâ€Principles Approach. ChemPhysChem, 2011, 12, 3157-3169.	1.0	8
98	Inside Cover: The Resonance Raman Spectra of Spheroidene Revisited with a Firstâ€Principles Approach (ChemPhysChem 17/2011). ChemPhysChem, 2011, 12, 3042-3042.	1.0	0
99	Linking the historical and chemical definitions of diabatic states for charge and excitation energy transfer reactions in condensed phase. Journal of Chemical Physics, 2011, 135, 134113.	1.2	18
100	Chromophore-specific theoretical spectroscopy: From subsystem density functional theory to mode-specific vibrational spectroscopy. Physics Reports, 2010, 489, 1-87.	10.3	118
101	Enhancement and de-enhancement effects in vibrational resonance Raman optical activity. Journal of Chemical Physics, 2010, 132, 044113.	1.2	55
102	Accurate frozen-density embedding potentials as a first step towards a subsystem description of covalent bonds. Journal of Chemical Physics, 2010, 132, 164101.	1.2	172
103	State-selective optimization of local excited electronic states in extended systems. Journal of Chemical Physics, 2010, 133, 174114.	1.2	19
104	A Subsystem TDDFT Approach for Solvent Screening Effects on Excitation Energy Transfer Couplings. Journal of Chemical Theory and Computation, 2010, 6, 1843-1851.	2.3	77
105	Phytochrome as Molecular Machine: Revealing Chromophore Action during the Pfr â†' Pr Photoconversion by Magic-Angle Spinning NMR Spectroscopy. Journal of the American Chemical Society, 2010, 132, 4431-4437.	6.6	55
106	On the calculation of general response properties in subsystem density functional theory. Journal of Chemical Physics, 2009, 131, 084104.	1.2	52
107	The electronic structure of the primary electron donor of reaction centers of purple bacteria at atomic resolution as observed by photo-CIDNP ¹³ C NMR. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 22281-22286.	3.3	74
108	Intensity tracking for theoretical infrared spectroscopy of large molecules. Journal of Chemical Physics, 2009, 130, 064105.	1.2	39

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109	Subsystemâ€Based Theoretical Spectroscopy of Biomolecules and Biomolecular Assemblies. ChemPhysChem, 2009, 10, 3148-3173.	1.0	91
110	Intensity Tracking for Vibrational Spectra of Large Molecules. Chimia, 2009, 63, 270-274.	0.3	16
111	A vibrational circular dichroism implementation within a Slater-type-orbital based density functional framework and its application to hexa- and hepta-helicenes. Theoretical Chemistry Accounts, 2008, 119, 245-263.	0.5	87
112	A flexible implementation of frozenâ€density embedding for use in multilevel simulations. Journal of Computational Chemistry, 2008, 29, 1011-1018.	1.5	138
113	QM/MM vibrational mode tracking. Journal of Computational Chemistry, 2008, 29, 2460-2470.	1.5	21
114	Analysis of electron density distributions from subsystem density functional theory applied to coordination bonds. Chemical Physics Letters, 2008, 461, 353-359.	1.2	66
115	Photophysical Properties of Natural Light-Harvesting Complexes Studied by Subsystem Density Functional Theory. Journal of Physical Chemistry B, 2008, 112, 2207-2217.	1.2	90
116	Topological analysis of electron densities from Kohn-Sham and subsystem density functional theory. Journal of Chemical Physics, 2008, 128, 044114.	1.2	56
117	Effects of Complex Formation on Vibrational Circular Dichroism Spectra. Journal of Physical Chemistry A, 2008, 112, 6978-6991.	1.1	73
118	Gas-Phase Cî”H and Nî”H Bond Activation by a High Valent Nitrido-Iron Dication and ã€ˆNHã€‰-Transfer to Activated Olefins. Journal of the American Chemical Society, 2008, 130, 4285-4294.	6.6	85
119	Selective calculation of high-intensity vibrations in molecular resonance Raman spectra. Journal of Chemical Physics, 2008, 129, 204103.	1.2	36
120	Finding a needle in a haystack: direct determination of vibrational signatures in complex systems. New Journal of Chemistry, 2007, 31, 818.	1.4	66
121	The First Photoexcitation Step of Ruthenium-Based Models for Artificial Photosynthesis Highlighted by Resonance Raman Spectroscopy. Journal of Physical Chemistry B, 2007, 111, 6078-6087.	1.2	57
122	Couplings between electronic transitions in a subsystem formulation of time-dependent density functional theory. Journal of Chemical Physics, 2007, 126, 134116.	1.2	214
123	Induced Chirality in Achiral Mediaâ€”How Theory Unravels Mysterious Solvent Effects. Angewandte Chemie - International Edition, 2007, 46, 7738-7740.	7.2	39
124	Comparison of frozen-density embedding and discrete reaction field solvent models for molecular properties. Physical Chemistry Chemical Physics, 2006, 8, 2349.	1.3	87
125	Exploring the Ability of Frozen-Density Embedding to Model Induced Circular Dichroism. Journal of Physical Chemistry A, 2006, 110, 8786-8796.	1.1	52
126	Assessment of a simple correction for the long-range charge-transfer problem in time-dependent density-functional theory. Journal of Chemical Physics, 2006, 124, 214102.	1.2	126

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127	The ?Invisible?13C NMR Chemical Shift of the Central Carbon Atom in [(Ph3PAu)6C]2+: A Theoretical Investigation. Chemistry - A European Journal, 2005, 11, 1677-1686.	1.7	15
128	Comment on â€œGradient-based direct normal-mode analysisâ€•[J. Chem. Phys. 122, 184106 (2005)]. Journal of Chemical Physics, 2005, 123, 117101.	1.2	9
129	Importance of vibronic effects on the circular dichroism spectrum of dimethyloxirane. Journal of Chemical Physics, 2005, 122, 234305.	1.2	54
130	The merits of the frozen-density embedding scheme to model solvatochromic shifts. Journal of Chemical Physics, 2005, 122, 094115.	1.2	207
131	Combined Theoretical and Experimental Deep-UV Resonance Raman Studies of Substituted Pyrenes. Journal of Physical Chemistry A, 2005, 109, 2100-2106.	1.1	59
132	An Explicit Quantum Chemical Method for Modeling Large Solvation Shells Applied to Aminocoumarin C151. Journal of Physical Chemistry A, 2005, 109, 7805-7814.	1.1	130
133	Vibronic Structure of the Permanganate Absorption Spectrum from Time-Dependent Density Functional Calculations. Journal of Physical Chemistry A, 2005, 109, 1168-1179.	1.1	65
134	Modeling solvent effects on electron-spin-resonance hyperfine couplings by frozen-density embedding. Journal of Chemical Physics, 2005, 123, 114101.	1.2	64
135	Theoretical Study on the Spin-State Energy Splittings and Local Spin in Cationic [Re]â˜Cnâ˜[Re] Complexes. Inorganic Chemistry, 2005, 44, 6174-6182.	1.9	28
136	Vibronic coupling and double excitations in linear response time-dependent density functional calculations: Dipole-allowed states of N2. Journal of Chemical Physics, 2004, 121, 6155-6166.	1.2	80
137	Resonance Raman spectra of uracil based on Kramersâ€“Kronig relations using time-dependent density functional calculations and multireference perturbation theory. Journal of Chemical Physics, 2004, 120, 11564-11577.	1.2	81
138	Vibrational center-ligand couplings in transition metal complexes. Journal of Computational Chemistry, 2004, 25, 587-597.	1.5	26
139	Properties of WAu12.. ChemInform, 2004, 35, no.	0.1	0
140	Properties of WAu12. Physical Chemistry Chemical Physics, 2004, 6, 11-22.	1.3	97
141	Convergence characteristics and efficiency of mode-tracking calculations on pre-selected molecular vibrations. Physical Chemistry Chemical Physics, 2004, 6, 4621.	1.3	39
142	Mode Tracking of Preselected Vibrations of One-Dimensional Molecular Wires. Journal of Physical Chemistry A, 2004, 108, 2053-2061.	1.1	31
143	Fundamental vibrational frequencies of small polyatomic molecules from density-functional calculations and vibrational perturbation theory. Journal of Chemical Physics, 2003, 118, 7215.	1.2	259
144	A mode-selective quantum chemical method for tracking molecular vibrations applied to functionalized carbon nanotubes. Journal of Chemical Physics, 2003, 118, 1634-1641.	1.2	106

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145	Analysis of the asymptotic and short-range behavior of quasilocal Hartree-Fock and Dirac-Fock-Coulomb electron-electron interaction potentials. Physical Review A, 2002, 65, .	1.0	9
146	Analytical local electron-electron interaction model potentials for atoms. Physical Review A, 2002, 66, .	1.0	7
147	Publisherâ€™s Note: Analytical local electron-electron interaction model potentials for atoms [Phys. Rev. A66, 022717 (2002)]. Physical Review A, 2002, 66, .	1.0	0
148	Coupled-cluster Raman intensities: Assessment and comparison with multiconfiguration and density functional methods. Journal of Chemical Physics, 2002, 117, 8623-8633.	1.2	39
149	Quantum chemical calculation of vibrational spectra of large molecules?Raman and IR spectra for Buckminsterfullerene. Journal of Computational Chemistry, 2002, 23, 895-910.	1.5	506
150	Orbital Pair Selection for Relative Energies in the Domain-Based Local Pair Natural Orbital Coupled-Cluster Method. Journal of Chemical Physics, 0, , .	1.2	3