Christoph R Jacob

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5376284/publications.pdf

Version: 2024-02-01

85	4,707	94269	95083
papers	citations	37 h-index	68 g-index

113	113	113	4214
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Systematic QM Region Construction in QM/MM Calculations Based on Uncertainty Quantification. Journal of Chemical Theory and Computation, 2022, 18, 2584-2596.	2.3	16
2	Systematic Partitioning of Proteins for Quantum-Chemical Fragmentation Methods Using Graph Algorithms. Journal of Chemical Theory and Computation, 2021, 17, 1355-1367.	2.3	4
3	Electrocatalytic Activation of Donorâ€“Acceptor Cyclopropanes and Cyclobutanes: An Alternative C(sp³)â^'C(sp³) Cleavage Mode. Angewandte Chemie - International Edition, 2021, 60, 15928-15934.	7.2	60
4	Electrocatalytic Activation of Donorâ€“Acceptor Cyclopropanes and Cyclobutanes: An Alternative C(sp³)â^'C(sp³) Cleavage Mode. Angewandte Chemie, 2021, 133, 16064-16070.	1.6	18
5	Density-Based Many-Body Expansion as an Efficient and Accurate Quantum-Chemical Fragmentation Method: Application to Water Clusters. Journal of Chemical Theory and Computation, 2021, 17, 4144-4156.	2.3	13
6	[(Me₃P)₃Co(Bcat)₃]: Equilibrium Oxidative Addition of a Bâ€“B Bond and Interconversion between the fac-Tris-Boryl and the mer-Tris-Boryl Complex. Organometallics, 2020, 39, 538-543.	1.1	9
7	Frozenâ€density embeddingâ€based manyâ€body expansions. International Journal of Quantum Chemistry, 2020, 120, e26228.	1.0	15
8	Challenges for large scale simulation: general discussion. Faraday Discussions, 2020, 224, 309-332.	1.6	2
9	New density-functional approximations and beyond: general discussion. Faraday Discussions, 2020, 224, 166-200.	1.6	1
10	Environmental Effects with Frozen-Density Embedding in Real-Time Time-Dependent Density Functional Theory Using Localized Basis Functions. Journal of Chemical Theory and Computation, 2020, 16, 5695-5711.	2.3	12
11	The DIRAC code for relativistic molecular calculations. Journal of Chemical Physics, 2020, 152, 204104.	1.2	191
12	Spin-state dependence of exchangeâ€“correlation holes. Faraday Discussions, 2020, 224, 56-78.	1.6	4
13	Electronic Structure of the Hieber Anion [Fe(CO)₃(NO)]^{â^'} Revisited by X-ray Emission and Absorption Spectroscopy. Inorganic Chemistry, 2020, 59, 3551-3561.	1.9	14
14	Towards theoretical spectroscopy with error bars: systematic quantification of the structural sensitivity of calculated spectra. Chemical Science, 2020, 11, 1862-1877.	3.7	13
15	A new ultrafast energy funneling material harvests three times more diffusive solar energy for GaInP photovoltaics. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 32929-32938.	3.3	2
16	Description of intermolecular charge transfer with subsystem density-functional theory. Journal of Chemical Physics, 2019, 151, 131103.	1.2	11
17	QMflows: A Tool Kit for Interoperable Parallel Workflows in Quantum Chemistry. Journal of Chemical Information and Modeling, 2019, 59, 3191-3197.	2.5	32
18	Computational Insights into the Mechanism of the Selective Catalytic Reduction of NOx: Fe- versus Cu-Exchanged Zeolite Catalysts. ACS Omega, 2019, 4, 7987-7993.	1.6	11

#	Article	IF	Citations
19	Position 123 of halohydrin dehalogenase HheG plays an important role in stability, activity, and enantioselectivity. Scientific Reports, 2019, 9, 5106.	1.6	12
20	On the choice of coordinates in anharmonic theoretical vibrational spectroscopy: Harmonic vs. anharmonic coupling in vibrational configuration interaction. Journal of Chemical Physics, 2019, 150, 054107.	1.2	21
21	Simulation of FRET dyes allows quantitative comparison against experimental data. Journal of Chemical Physics, 2018, 148, 123321.	1.2	39
22	Uncertainty quantification in theoretical spectroscopy: The structural sensitivity of Xâ€ray emission spectra. International Journal of Quantum Chemistry, 2018, 118, e25458.	1.0	8
23	Revisiting the Dependence of Cu K-Edge X-ray Absorption Spectra on Oxidation State and Coordination Environment. Inorganic Chemistry, 2018, 57, 10591-10607.	1.9	29
24	Differences in the complexation of sodium with methyl esterified carboxymethyl/methoxyacetyl-O-glucans in electrospray ionization-mass spectrometry. International Journal of Mass Spectrometry, 2017, 419, 20-28.	0.7	7
25	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
26	Theoretische RÃ¶ntgenspektroskopie. Nachrichten Aus Der Chemie, 2016, 64, 325-327.	0.0	0
27	On the benefits of localized modes in anharmonic vibrational calculations for small molecules. Journal of Chemical Physics, 2016, 144, 164111.	1.2	33
28	Anharmonic Theoretical Vibrational Spectroscopy of Polypeptides. Journal of Physical Chemistry Letters, 2016, 7, 3084-3090.	2.1	37
29	Towards advanced structural analysis of iron oxide clusters on the surface of Î³-Al2O3 using EXAFS. Applied Surface Science, 2016, 386, 234-246.	3.1	14
30	How Open Is Commercial Scientific Software?. Journal of Physical Chemistry Letters, 2016, 7, 351-353.	2.1	14
31	No need for external orthogonality in subsystem density-functional theory. Physical Chemistry Chemical Physics, 2016, 18, 21001-21009.	1.3	21
32	Better Partitions of Protein Graphs for Subsystem Quantum Chemistry. Lecture Notes in Computer Science, 2016, , 353-368.	1.0	6
33	Excitation energies from frozen-density embedding with accurate embedding potentials. Journal of Chemical Physics, 2015, 142, 234101.	1.2	23
34	Methanolâ€induced change of the mechanism of the temperatureâ€and pressureâ€induced collapse of Nâ€Substituted acrylamide copolymers. Journal of Polymer Science, Part B: Polymer Physics, 2015, 53, 532-544.	2.4	9
35	High-resolution X-ray absorption spectroscopy of iron carbonyl complexes. Physical Chemistry Chemical Physics, 2015, 17, 13937-13948.	1.3	36
36	Structural snapshots of the SCR reaction mechanism on Cu-SSZ-13. Chemical Communications, 2015, 51, 9227-9230.	2.2	101

#	Article	IF	Citations
37	Identification of Plasmons in Molecules with Scaled Ab Initio Approaches. Journal of Physical Chemistry C, 2015, 119, 24564-24573.	1.5	34
38	Plasmons in molecules: Microscopic characterization based on orbital transitions and momentum conservation. Journal of Chemical Physics, 2014, 141, 104101.	1.2	26
39	Subsystem densityâ€functional theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 325-362.	6.2	282
40	Efficient Calculation of Anharmonic Vibrational Spectra of Large Molecules with Localized Modes. ChemPhysChem, 2014, 15, 3365-3377.	1.0	65
41	Ion Mobility Spectrometry, Infrared Dissociation Spectroscopy, and ab Initio Computations toward Structural Characterization of the Deprotonated Leucine-Enkephalin Peptide Anion in the Gas Phase. Journal of Physical Chemistry A, 2014, 118, 8453-8463.	1.1	13
42	Selective Catalytic Reduction of NO Over Fe-ZSM-5: Mechanistic Insights by Operando HERFD-XANES and Valence-to-Core X-ray Emission Spectroscopy. Journal of the American Chemical Society, 2014, 136, 13006-13015.	6.6	128
43	Epitaxial Growth of Pentacene on Alkali Halide Surfaces Studied by Kelvin Probe Force Microscopy. ACS Nano, 2014, 8, 3294-3301.	7.3	22
44	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
45	Towards systematically improvable models for actinides in condensed phase: the electronic spectrum of uranyl in Cs2UO2Cl4 as a test case. Physical Chemistry Chemical Physics, 2013, 15, 15153.	1.3	44
46	Plasmons in Molecules. Journal of Physical Chemistry C, 2013, 117, 1863-1878.	1.5	121
47	Optimized unrestricted Kohnâ€“Sham potentials from ab initio spin densities. Journal of Chemical Physics, 2013, 138, 044111.	1.2	25
48	The chemical sensitivity of X-ray spectroscopy: high energy resolution XANES versus X-ray emission spectroscopy of substituted ferrocenes. Physical Chemistry Chemical Physics, 2013, 15, 8095.	1.3	52
49	Quantum-Chemical Electron Densities of Proteins and of Selected Protein Sites from Subsystem Density Functional Theory. Journal of Chemical Theory and Computation, 2013, 9, 2425-2440.	2.3	43
50	Towards the Description of Covalent Bonds in Subsystem Density-Functional Theory. Recent Advances in Computational, 2013, , 297-322.	0.8	5
51	Quantum-chemical embedding methods for treating local electronic excitations in complex chemical systems. Annual Reports on the Progress of Chemistry Section C, 2012, 108, 222.	4.4	183
52	Spin in densityâ€functional theory. International Journal of Quantum Chemistry, 2012, 112, 3661-3684.	1.0	185
53	Origin-independent calculation of quadrupole intensities in X-ray spectroscopy. Journal of Chemical Physics, 2012, 137, 204106.	1.2	83
54	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

#	Article	IF	Citations
55	Probing the Electronic Structure of Substituted Ferrocenes with Highâ€Resolution XANES Spectroscopy. Chemistry - A European Journal, 2012, 18, 7021-7025.	1.7	41
56	Analysis of the Cartesian Tensor Transfer Method for Calculating Vibrational Spectra of Polypeptides. Journal of Chemical Theory and Computation, 2011, 7, 1867-1881.	2.3	46
57	Can DFT Accurately Predict Spin Densities? Analysis of Discrepancies in Iron Nitrosyl Complexes. Journal of Chemical Theory and Computation, 2011, 7, 2740-2752.	2.3	96
58	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
59	Identifying Protein Î²-Turns with Vibrational Raman Optical Activity. ChemPhysChem, 2011, 12, 1165-1175.	1.0	13
60	Theoretical Study of the Raman Optical Activity Spectra of 3₁₀â€Helical Polypeptides. ChemPhysChem, 2011, 12, 3291-3306.	1.0	19
61	PyADF â€” A scripting framework for multiscale quantum chemistry. Journal of Computational Chemistry, 2011, 32, 2328-2338.	1.5	71
62	Unambiguous optimization of effective potentials in finite basis sets. Journal of Chemical Physics, 2011, 135, 244102.	1.2	58
63	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
64	Raman Optical Activity Study of the Signatures Associated to (TG)[sub N] and (GG)[sub N] Conformations of Isotactic Polypropylene Chains using Mode Localization Method. , 2010, , .		1
65	The weak covalent bond in NgAuF (Ng=Ar, Kr, Xe): A challenge for subsystem density functional theory. Journal of Chemical Physics, 2010, 132, 044114.	1.2	41
66	Analysis of Vibrational Raman Optical Activity Signatures of the (TG)N and (GG)N Conformations of Isotactic Polypropylene Chains in Terms of Localized Modes. Journal of Physical Chemistry A, 2010, 114, 7198-7212.	1.1	21
67	A Local-Mode Model for Understanding the Dependence of the Extended Amide III Vibrations on Protein Secondary Structure. Journal of Physical Chemistry B, 2010, 114, 10649-10660.	1.2	55
68	Understanding the Signatures of Secondaryâ€Structure Elements in Proteins with Raman Optical Activity Spectroscopy. Chemistry - A European Journal, 2009, 15, 13491-13508.	1.7	67
69	Localizing normal modes in large molecules. Journal of Chemical Physics, 2009, 130, 084106.	1.2	140
70	Analysis of Secondary Structure Effects on the IR and Raman Spectra of Polypeptides in Terms of Localized Vibrations. Journal of Physical Chemistry B, 2009, 113, 6558-6573.	1.2	72
71	Calculated Raman Optical Activity Signatures of Tryptophan Side Chains. ChemPhysChem, 2008, 9, 2177-2180.	1.0	48
72	A flexible implementation of frozenâ€density embedding for use in multilevel simulations. Journal of Computational Chemistry, 2008, 29, 1011-1018.	1.5	138

#	Article	IF	Citations
73	Analysis of electron density distributions from subsystem density functional theory applied to coordination bonds. Chemical Physics Letters, 2008, 461, 353-359.	1.2	66
74	NMR Solvent Shifts of Acetonitrile from Frozen Density Embedding Calculations. Journal of Physical Chemistry A, 2008, 112, 2640-2647.	1.1	42
75	A subsystem density-functional theory approach for the quantum chemical treatment of proteins. Journal of Chemical Physics, 2008, 128, 155102.	1.2	88
76	Calculation of local excitations in large systems by embedding wave-function theory in density-functional theory. Physical Chemistry Chemical Physics, 2008, 10, 5353.	1.3	145
77	The adsorption of CO on charged and neutral Au and Au2: A comparison between wave-function based and density functional theory. Journal of Chemical Physics, 2008, 128, 124302.	1.2	27
78	Nuclear quadrupole moment of La139 from relativistic electronic structure calculations of the electric field gradients in LaF, LaCl, LaBr, and LaI. Journal of Chemical Physics, 2007, 127, 204303.	1.2	14
79	Exact functional derivative of the nonadditive kinetic-energy bifunctional in the long-distance limit. Journal of Chemical Physics, 2007, 126, 234116.	1.2	68
80	Comparison of frozen-density embedding and discrete reaction field solvent models for molecular properties. Physical Chemistry Chemical Physics, 2006, 8, 2349.	1.3	87
81	Calculation of nuclear magnetic resonance shieldings using frozen-density embedding. Journal of Chemical Physics, 2006, 125, 194104.	1.2	69
82	Orbital-free embedding applied to the calculation of induced dipole moments in CO2â‹¯X (X=He, Ne, Ar, Kr,) Tj ETQq0 0 0 rgBT /Overlock	1.2	61
83	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
84	The quadrupole moment of the 3âˆ•2+ nuclear ground state of Au197 from electric field gradient relativistic coupled cluster and density-functional theory of small molecules and the solid state. Journal of Chemical Physics, 2005, 122, 124317.	1.2	37
85	The structures of small gold cluster anions as determined by a combination of ion mobility measurements and density functional calculations. Journal of Chemical Physics, 2002, 117, 6982-6990.	1.2	524