JÃ¡nos ÃngyÃ¡n

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3346806/publications.pdf

Version: 2024-02-01

132	10,509	50273	31843
papers	citations	46 h-index	101 g-index

133	133	133	9601
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Screened hybrid density functionals applied to solids. Journal of Chemical Physics, 2006, 124, 154709.	3.0	1,915
2	Improved Description of the Structure of Molecular and Layered Crystals: Ab Initio DFT Calculations with van der Waals Corrections. Journal of Physical Chemistry A, 2010, 114, 11814-11824.	2.5	895
3	Assessing the performance of recent density functionals for bulk solids. Physical Review B, 2009, 79, .	3.2	740
4	Cohesive Properties and Asymptotics of the Dispersion Interaction in Graphite by the Random Phase Approximation. Physical Review Letters, 2010, 105, 196401.	7.8	330
5	Covalent Bond Orders and Atomic Valence Indices in the Topological Theory of Atoms in Molecules. The Journal of Physical Chemistry, 1994, 98, 5244-5248.	2.9	290
6	van der Waals forces in density functional theory: Perturbational long-range electron-interaction corrections. Physical Review A, 2005, 72, .	2.5	287
7	Peptide models. 1. Topology of selected peptide conformational potential energy surfaces (glycine and) Tj ETQq1 1 0.784314 rgBT /Ove	13.7	244
8	Hybrid functional with separated range. Chemical Physics Letters, 2005, 415, 100-105.	2.6	243
9	Adiabatic-Connection Fluctuation-Dissipation Density-Functional Theory Based on Range Separation. Physical Review Letters, 2009, 102, 096404.	7.8	240
10	Improved Density Dependent Correction for the Description of London Dispersion Forces. Journal of Chemical Theory and Computation, 2013, 9, 4293-4299.	5.3	183
11	Polymorphism in silica studied in the local density and generalized-gradient approximations. Journal of Physics Condensed Matter, 1999, 11, 3833-3874.	1.8	174
12	Extending the applicability of the Tkatchenko-Scheffler dispersion correction via iterative Hirshfeld partitioning. Journal of Chemical Physics, 2014, 141, 034114.	3.0	174
13	BrÃ¸nsted Acid Sites in HSAPO-34 and Chabazite:â€‰ An Ab Initio Structural Study. Journal of Physical Chemistry B, 1998, 102, 5573-5580.	2.6	166
14	Chalcogen Bonding: Experimental and Theoretical Determinations from Electron Density Analysis. Geometrical Preferences Driven by Electrophilicâ€“Nucleophilic Interactions. Crystal Growth and Design, 2013, 13, 3283-3289.	3.0	154
15	Distributed polarizabilities using the topological theory of atoms in molecules. Chemical Physics Letters, 1994, 219, 267-273.	2.6	142
16	Geometry optimization of periodic systems using internal coordinates. Journal of Chemical Physics, 2005, 122, 124508.	3.0	128
17	Bonding between nonbonded sulfur and oxygen atoms in selected organic molecules (a quantum) Tj ETQq1 1 0.784314 rgBT /Overlo	13.7	123
18	Correlation Energy Expressions from the Adiabatic-Connection Fluctuationâ€“Dissipation Theorem Approach. Journal of Chemical Theory and Computation, 2011, 7, 3116-3130.	5.3	122

#	Article	IF	Citations
19	Range-separated density-functional theory with random phase approximation applied to noncovalent intermolecular interactions. Journal of Chemical Physics, 2010, 132, 244108.	3.0	119
20	Range-separated density-functional theory with the random-phase approximation: Detailed formalism and illustrative applications. Physical Review A, 2010, 82, .	2.5	115
21	Monomolecular cracking of propane over acidic chabazite: An ab initio molecular dynamics and transition path sampling study. Journal of Catalysis, 2011, 279, 220-228.	6.2	98
22	Blind test of density-functional-based methods on intermolecular interaction energies. Journal of Chemical Physics, 2016, 145, 124105.	3.0	97
23	Comparison of ab Initio Hartreeâ^'Fock and Kohnâ^'Sham Orbitals in the Calculation of Atomic Charge, Bond Index, and Valence. Journal of Physical Chemistry A, 2000, 104, 9953-9963.	2.5	93
24	Approximate electrostatic interaction operator for QM/MM calculations. Chemical Physics Letters, 2002, 356, 331-339.	2.6	92
25	A Fractionally Ionic Approach to Polarizability and van der Waals Many-Body Dispersion Calculations. Journal of Chemical Theory and Computation, 2016, 12, 5920-5930.	5.3	90
26	Range separated hybrid density functional with long-range Hartree-Fock exchange applied to solids. Journal of Chemical Physics, 2007, 127, 054101.	3.0	89
27	The origin of the problems with the PM3 core repulsion function. Computational and Theoretical Chemistry, 1997, 393, 31-38.	1.5	88
28	Many-body dispersion corrections for periodic systems: an efficient reciprocal space implementation. Journal of Physics Condensed Matter, 2016, 28, 045201.	1.8	86
29	Reaction field factors for a multipole distribution in a cavity surrounded by a continuum. Chemical Physics Letters, 1993, 202, 18-22.	2.6	85
30	Closed-shell ring coupled cluster doubles theory with range separation applied on weak intermolecular interactions. Journal of Chemical Physics, 2011, 135, 084119.	3.0	85
31	Charge Density Analysis and Topological Properties of Hal₃-Synthons and Their Comparison with Competing Hydrogen Bonds. Crystal Growth and Design, 2012, 12, 5373-5386.	3.0	78
32	Effect of Polarizability on the Potential of Mean Force of Two Cations. The Guanidiniumâ^'Guanidinium Ion Pair in Water. Journal of Physical Chemistry B, 1997, 101, 10910-10917.	2.6	77
33	Modeling spin-crossover compounds by periodic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>DFT</mml:mtext><mml:mo>+</mml:mo><mml:mtext>U</mml:mtext></mml:mrow></mml Physical Review B, 2008, 78, .	3.2	76
34	On the equivalence of ring-coupled cluster and adiabatic connection fluctuation-dissipation theorem random phase approximation correlation energy expressions. Journal of Chemical Physics, 2010, 133, 154106.	3.0	75
35	Transferable net atomic charges from a distributed multipole analysis for the description of electrostatic properties: a case study of saturated hydrocarbons. The Journal of Physical Chemistry, 1993, 97, 6628-6636.	2.9	74
36	Choosing between alternative MP2 algorithms in the self-consistent reaction field theory of solvent effects. Chemical Physics Letters, 1995, 241, 51-56.	2.6	72

#	Article	IF	Citations
37	Distributed polarizability of the water dimer: Field-induced charge transfer along the hydrogen bond. Journal of Chemical Physics, 2001, 114, 7951-7961.	3.0	70
38	Common theoretical framework for quantum chemical solvent effect theories. Journal of Mathematical Chemistry, 1992, 10, 93-137.	1.5	65
39	Covalent bond orders and atomic valences from correlated wavefunctions. Chemical Physics Letters, 1999, 299, 1-8.	2.6	60
40	Spin crossover transition of Fe(phen)2(NCS)2: periodic dispersion-corrected density-functional study. Physical Chemistry Chemical Physics, 2012, 14, 5389.	2.8	57
41	On the Nature of Water Interacting with BrÃ¸nsted Acidic Sites. Ab Initio Molecular Dynamics Study of Hydrated HSAPO-34. Journal of Physical Chemistry B, 1998, 102, 7307-7310.	2.6	56
42	Distributed first and second order hyperpolarizabilities: An improved calculation of nonlinear optical susceptibilities of molecular crystals. Journal of Chemical Physics, 2000, 112, 6161-6172.	3.0	55
43	Quantum-chemical model calculations on the acidic site of zeolites including Madelung-potential effects. Chemical Physics Letters, 1990, 168, 461-467.	2.6	54
44	Potential curves for alkaline-earth dimers by density functional theory with long-range correlation corrections. Chemical Physics Letters, 2005, 416, 370-375.	2.6	52
45	On the exchange-hole model of London dispersion forces. Journal of Chemical Physics, 2007, 127, 024108.	3.0	51
46	Proton exchange of small hydrocarbons over acidic chabazite: Ab initio study of entropic effects. Journal of Catalysis, 2007, 250, 171-183.	6.2	51
47	A comprehensive approach to molecular charge density models: From distributed multipoles to fitted atomic charges. International Journal of Quantum Chemistry, 1994, 52, 17-37.	2.0	47
48	Intermolecular interaction energies by topologically partitioned electric properties II. Dispersion energies in one-centre and multicentre multipole expansions. Molecular Physics, 1997, 91, 145-160.	1.7	45
49	Periodic Projector Augmented Wave Density Functional Calculations on the Hexachlorobenzene Crystal and Comparison with the Experimental Multipolar Charge Density Model. Journal of Physical Chemistry A, 2011, 115, 14484-14494.	2.5	43
50	Electrostatic interactions in threeâ€dimensional solids. Selfâ€consistent Madelung potential (SCMP) approach. Journal of Chemical Physics, 1987, 86, 6957-6966.	3.0	41
51	Derivation of Distributed Models of Atomic Polarizability for Molecular Simulations. Journal of Chemical Theory and Computation, 2007, 3, 1901-1913.	5.3	41
52	Ab Initio Study of Structure and Interconversion of Native Cellulose Phases. Journal of Physical Chemistry A, 2011, 115, 10097-10105.	2.5	41
53	Distributed polarizabilities derived from induction energies: A finite perturbation approach. Journal of Chemical Physics, 2000, 112, 2709-2717.	3.0	40
54	Rayleigh-SchrÃ¶dinger perturbation theory for nonlinear SchrÃ¶dinger equations with linear perturbation. International Journal of Quantum Chemistry, 1993, 47, 469-483.	2.0	39

#	Article	IF	Citations
55	OPEP: A tool for the optimal partitioning of electric properties. Journal of Computational Chemistry, 2003, 24, 997-1008.	3.3	39
56	Comparison of protein electrostatic potential along the catalytic triad of serine proteinases. Journal of Theoretical Biology, 1983, 103, 349-356.	1.7	38
57	Molecular electrostatic fields from bond fragments. International Journal of Quantum Chemistry, 1987, 31, 927-939.	2.0	38
58	Aurophilic Interactions from Wave Function, Symmetry-Adapted Perturbation Theory, and Rangehybrid Approaches. Journal of Chemical Theory and Computation, 2011, 7, 2399-2407.	5.3	37
59	Generalized self-consistent reaction field theory in a multicenter-multipole ab-initio LCGO framework. I. Electronic properties of the water molecule in a Monte Carlo sample of liquid water molecules studied with standard basis sets. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1990, 87, 875-903.	0.2	37
60	A SCRFâ€CNDO/2 study on proton conductivity mechanisms in hydronium perchlorate. Towards a quantum chemical representation of defects and impurities in crystals. Journal of Chemical Physics, 1982, 77, 4723-4733.	3.0	36
61	Perturbation theory for nonlinear time-independent SchrÃ¶dinger equations. Physical Review A, 1983, 28, 45-48.	2.5	35
62	Statistical analysis of distributed multipoles derived from molecular electrostatic potentials. Molecular Physics, 1998, 94, 881-895.	1.7	35
63	Crystal and electronic structure of two polymorphic modifications of famotidine. An experimental and theoretical study. Computational and Theoretical Chemistry, 2000, 503, 73-79.	1.5	35
64	Modeling Induction Phenomena in Intermolecular Interactions with an Ab Initio Force Field. Journal of Chemical Theory and Computation, 2007, 3, 1914-1926.	5.3	34
65	Spin-unrestricted random-phase approximation with range separation: Benchmark on atomization energies and reaction barrier heights. Journal of Chemical Physics, 2015, 142, 154123.	3.0	34
66	Intermolecular interaction energies by topologically partitioned electric properties. 1. Electrostatic and induction energies in one-centre and multicentre multipole expansions. Molecular Physics, 1996, 88, 69-92.	1.7	34
67	Fast and accurate determination of induction energies: reduction of topologically distributed polarizability models. Chemical Physics Letters, 2001, 338, 180-188.	2.6	32
68	Dielectric Matrix Formulation of Correlation Energies in the Random Phase Approximation: Inclusion of Exchange Effects. Journal of Chemical Theory and Computation, 2016, 12, 2191-2202.	5.3	31
69	Critical analysis of electric field modeling: Formamide. Journal of Computational Chemistry, 1992, 13, 1234-1245.	3.3	30
70	Modeling amino acid side chains. 2. Determination of point charges from electrostatic properties: toward transferable point charge models. The Journal of Physical Chemistry, 1993, 97, 9788-9796.	2.9	30
71	Transferability of topologically partitioned polarizabilities: the case of n-alkanes. Molecular Physics, 1996, 89, 595-605.	1.7	29
72	Short range DFT combined with long-range local RPA within a range-separated hybrid DFT framework. Chemical Physics Letters, 2012, 550, 162-169.	2.6	29

#	Article	IF	Citations
73	Ab initio and DFT investigations of intramolecular hydrogen bonding in 1,2-ethanediol. Chemical Physics Letters, 1995, 245, 129-135.	2.6	28
74	The Black Polymorph of TTF-CA: TTF Polymorphism and Solvent Effects in Mechanochemical and Vapor Digestion Syntheses, FT-IR, Crystal Packing, and Electronic Structure. Crystal Growth and Design, 2014, 14, 91-100.	3.0	28
75	Linear scaling algorithm for the coordinate transformation problem of molecular geometry optimization. Journal of Chemical Physics, 2000, 113, 5598-5603.	3.0	27
76	Noncovalent structural models for the Asp-His dyad in the active site of serine proteases and for solid-state switching of protonation states: crystal structure of the associates of 1,1'-binaphthyl-2,2'-dicarboxylic acid with imidazole in dihydrated and in anhydrous forms. Journal of the American Chemical Society, 1986, 108, 1275-1281.	13.7	26
77	Dispersion interaction in hydrogen-chain models. Journal of Chemical Physics, 2011, 134, 114106.	3.0	26
78	Topologically partitioned dynamic polarizabilities using the theory of atoms in molecules. Canadian Journal of Chemistry, 1996, 74, 976-987.	1.1	25
79	Rayleigh-SchrÃ¶dinger many-body perturbation theory for density functionals: A unified treatment of one- and two-electron perturbations. Physical Review A, 2008, 78, .	2.5	25
80	Intramolecular sulfurâ€"oxygen interaction: An ab initio conformational study of (Z)-3-fluorothio-2-propenal. Computational and Theoretical Chemistry, 1985, 123, 189-201.	1.5	23
81	Analytical first and second energy derivatives in the polarization model. Chemical Physics Letters, 1990, 166, 180-188.	2.6	23
82	Mixed quantum?classical calculations on the water molecule in liquid phase: Influence of a polarizable environment on electronic properties. International Journal of Quantum Chemistry, 1996, 58, 251-265.	2.0	23
83	Alternative Approaches for the Calculation of Induction Energies:Â Characterization, Effectiveness, and Pitfalls. Journal of Physical Chemistry A, 2001, 105, 11505-11514.	2.5	23
84	Performance of Cu^{II}â€, Pb^{II}â€, and Hg^{II}â€Exchanged Mordenite in the Adsorption of I₂, ICH₃, H₂O, CO, ClCH₃, and Cl₂: A Density Functional Study. ChemPhysChem, 2017, 18, 1642-1652.	2.1	23
85	A study on the backbone/side-chain interaction in N-formyl-(L)serineamide. Canadian Journal of Chemistry, 1990, 68, 1882-1888.	1.1	21
86	Modeling amino acid side chains. 3. Influence of intra- and intermolecular environment on point charges. The Journal of Physical Chemistry, 1993, 97, 9797-9807.	2.9	21
87	The reliability of the point charge model representing intermolecular effects in ab initio calculations. Chemical Physics Letters, 1994, 225, 258-264.	2.6	21
88	Determination of Distributed Polarizabilities from a Statistical Analysis of Induction Energies. Journal of Physical Chemistry A, 2000, 104, 1293-1303.	2.5	21
89	Analytical Energy Gradients in Range-Separated Hybrid Density Functional Theory with Random Phase Approximation. Journal of Chemical Theory and Computation, 2014, 10, 1968-1979.	5.3	21
90	Assessment of range-separated time-dependent density-functional theory for calculating C6 dispersion coefficients. Journal of Chemical Physics, 2013, 138, 194106.	3.0	20

#	Article	IF	Citations
91	Are direct reaction field methods appropriate for describing dispersion interactions?. Chemical Physics Letters, 1990, 175, 313-318.	2.6	19
92	Continuing challenges in the parametrization of intermolecular force fields. Towards an accurate description of electrostatic and induction terms. New Journal of Chemistry, 2005, 29, 411-420.	2.8	19
93	The use of theoretical indices for the characterization of Sî—¸O linkage multiplicity. Computational and Theoretical Chemistry, 1988, 165, 273-287.	1.5	18
94	Modelling the electric field of water obtained from accurate SCF wave functions. Chemical Physics Letters, 1990, 172, 55-61.	2.6	18
95	An efficient method for the coordinate transformation problem of massively three-dimensional networks. Journal of Chemical Physics, 2001, 114, 9747-9753.	3.0	18
96	Linear Response and Measures of Electron Delocalization in Molecules. Current Organic Chemistry, 2011, 15, 3609-3618.	1.6	18
97	Improving the accuracy of ground-state correlation energies within a plane-wave basis set: The electron-hole exchange kernel. Journal of Chemical Physics, 2016, 145, 104105.	3.0	18
98	Comment on â€œNew strategies to incorporate the solvent polarization in self-consistent reaction field and free-energy perturbation simulationsâ€•[J. Chem. Phys. 103, 10183 (1995)]. Journal of Chemical Physics, 1997, 107, 1291-1292.	3.0	16
99	Surface modification by substitution. Chemical Physics Letters, 1987, 136, 1-8.	2.6	15
100	Spherical harmonic expansion of short-range screened Coulomb interactions. Journal of Physics A, 2006, 39, 8613-8630.	1.6	15
101	OSIPE â€” a tool for scientific programming in FORTRAN. Computer Physics Communications, 1994, 81, 293-317.	7.5	14
102	Intra- and intermolecular interactions in crystals of polar molecules. A study by the mixed quantum mechanical/molecular mechanical SCMP-NDDO method. Journal of Computational Chemistry, 2001, 22, 1679-1690.	3.3	14
103	Charge density reconstitution from approximate exchange-correlation holes. Canadian Journal of Chemistry, 2009, 87, 1444-1450.	1.1	14
104	Normalization corrections to perturbation theory for the time-independent nonlinear SchrÃ¶dinger equation. Physical Review A, 1991, 44, 2188-2191.	2.5	13
105	Colour Polymorphism of a Bis(quinoxaline) Compound. European Journal of Organic Chemistry, 1999, 1999, 2119-2125.	2.4	13
106	Intermolecular Interaction Energies from Experimental Charge Density Studies. , 2011, , 387-433.		13
107	Bond orders in three-centre bonds. Computational and Theoretical Chemistry, 1989, 186, 61-67.	1.5	12
108	Theoretical CD spectrum calculations of the crown-ether aralkyl-ammonium salt complex. Chirality, 2002, 14, 377-385.	2.6	12

#	Article	IF	Citations
109	Wignerâ€™s (2nÂ+Â1) rule for nonlinear SchrÃ¶dinger equations. Journal of Mathematical Chemistry, 2009, 46, 1-14.	1.5	12
110	Calculations on electrostatic properties of HY zeolite. Journal of the Chemical Society, Faraday Transactions, 1990, 86, 3461-3466.	1.7	11
111	Calculation of electrostatic potentials and fields inside zeolite cavities. Collection of Czechoslovak Chemical Communications, 1988, 53, 2308-2319.	1.0	10
112	Correlation of bond orders and softnesses. Computational and Theoretical Chemistry, 2000, 501-502, 379-388.	1.5	10
113	Casimirâ€“Polder Size Consistency: A Constraint Violated by Some Dispersion Theories. Journal of Chemical Theory and Computation, 2017, 13, 5829-5833.	5.3	8
114	The role of optimum supplementary d-orbitals for hypervalent selenium compounds. Chemical Physics Letters, 1986, 131, 247-251.	2.6	7
115	Chemical building blocks in quantum chemical calculations. Perspective on "The density matrix in many-electron quantum mechanics I. Generalized product functions. Factorization and physical interpretation of the density matrices". Theoretical Chemistry Accounts, 2000, 103, 238-241.	1.4	7
116	Electrostatic complementarity in molecular aggregates. Computational and Theoretical Chemistry, 1987, 149, 169-176.	1.5	6
117	The role of induction forces in infra-red matrix shifts: quantum chemical calculations with reaction field model hamiltonian. Computational and Theoretical Chemistry, 1991, 232, 97-110.	1.5	6
118	Ab initio determination of electronic energy splitting and transition rates for imidogen in argon matrixes. The Journal of Physical Chemistry, 1993, 97, 10011-10020.	2.9	6
119	Relationships between charge density response functions, exchange holes and localized orbitals. Computational and Theoretical Chemistry, 2015, 1053, 44-52.	2.5	6
120	Assessment of a range-separated orbital-optimised random-phase approximation electron correlation method. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	6
121	Chemical Fragmentation Approach to the Quantum Chemical Description of Extended Systems. , 1991, , 1-49.		6
122	Intramolecular sulfur-oxygen interaction in sulfonium compounds and sulfoxides. Computational and Theoretical Chemistry, 1989, 186, 53-60.	1.5	5
123	Protein electrostatics on personal computers. Computational and Theoretical Chemistry, 1992, 256, 113-123.	1.5	5
124	Spooky correlations and unusual van der Waals forces between gapless and near-gapless molecules. Journal of Chemical Physics, 2016, 145, 204107.	3.0	5
125	Synthesis of Vinca alkaloids and related compounds. Part 18. Stereochemical investigations on some intermediates leading to (+)-vincamine. Journal of the Chemical Society Perkin Transactions II, 1984, , 1629-1636.	0.9	4
126	Structure and ring inversion of 2-pyrrolidone. Semiempirical quantum chemical study and analysis of X-ray data. Collection of Czechoslovak Chemical Communications, 1986, 51, 249-263.	1.0	3

#	Article	IF	Citations
127	Computational chemistry on a PC. International Journal of Quantum Chemistry, 1990, 38, 163-171.	2.0	3
128	Local random phase approximation with projected oscillator orbitals. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	3
129	Ab Initio Simulations of Zeolite Reactivity. Progress in Theoretical Chemistry and Physics, 2001, , 77-108.	0.2	3
130	Ab initio quantum chemical study of the structure and vibrational spectra of the vinylene carbonate molecule. The Journal of Physical Chemistry, 1986, 90, 6420-6424.	2.9	2
131	Chemical Fragmentation Approach to the Quantum Chemical Description of Extended Systems. , 1991, , 1-49.		2
132	Continuing Challenges in the Parametrization of Intermolecular Force Fields. Towards an Accurate Description of Electrostatic and Induction Terms. ChemInform, 2005, 36, no.	0.0	0