

Jnos ngyn

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131
papers

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h-index

93
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133
ext. papers

9,775
ext. citations

3.6
avg, IF

5.99
L-index

#	Paper	IF	Citations
131	Screened hybrid density functionals applied to solids. <i>Journal of Chemical Physics</i> , 2006 , 124, 154709	3.9	1591
130	Improved description of the structure of molecular and layered crystals: ab initio DFT calculations with van der Waals corrections. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 11814-24	2.8	737
129	Assessing the performance of recent density functionals for bulk solids. <i>Physical Review B</i> , 2009 , 79,	3.3	530
128	Cohesive properties and asymptotics of the dispersion interaction in graphite by the random phase approximation. <i>Physical Review Letters</i> , 2010 , 105, 196401	7.4	298
127	Covalent Bond Orders and Atomic Valence Indices in the Topological Theory of Atoms in Molecules. <i>The Journal of Physical Chemistry</i> , 1994 , 98, 5244-5248		269
126	van der Waals forces in density functional theory: Perturbational long-range electron-interaction corrections. <i>Physical Review A</i> , 2005 , 72,	2.6	265
125	Peptide models. 1. Topology of selected peptide conformational potential energy surfaces (glycine and alanine derivatives). <i>Journal of the American Chemical Society</i> , 1991 , 113, 6256-6265	16.4	233
124	Hybrid functional with separated range. <i>Chemical Physics Letters</i> , 2005 , 415, 100-105	2.5	227
123	Adiabatic-connection fluctuation-dissipation density-functional theory based on range separation. <i>Physical Review Letters</i> , 2009 , 102, 096404	7.4	222
122	Polymorphism in silica studied in the local density and generalized-gradient approximations. <i>Journal of Physics Condensed Matter</i> , 1999 , 11, 3833-3874	1.8	157
121	Brønsted Acid Sites in HSAPO-34 and Chabazite: An Ab Initio Structural Study. <i>Journal of Physical Chemistry B</i> , 1998 , 102, 5573-5580	3.4	146
120	Improved Density Dependent Correction for the Description of London Dispersion Forces. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 4293-9	6.4	138
119	Distributed polarizabilities using the topological theory of atoms in molecules. <i>Chemical Physics Letters</i> , 1994 , 219, 267-273	2.5	136
118	Extending the applicability of the Tkatchenko-Scheffler dispersion correction via iterative Hirshfeld partitioning. <i>Journal of Chemical Physics</i> , 2014 , 141, 034114	3.9	134
117	Chalcogen Bonding: Experimental and Theoretical Determinations from Electron Density Analysis. Geometrical Preferences Driven by Electrophilic-Nucleophilic Interactions. <i>Crystal Growth and Design</i> , 2013 , 13, 3283-3289	3.5	134
116	Range-separated density-functional theory with random phase approximation applied to noncovalent intermolecular interactions. <i>Journal of Chemical Physics</i> , 2010 , 132, 244108	3.9	113
115	Bonding between nonbonded sulfur and oxygen atoms in selected organic molecules (a quantum chemical study). <i>Journal of the American Chemical Society</i> , 1987 , 109, 2237-2245	16.4	109

114	Geometry optimization of periodic systems using internal coordinates. <i>Journal of Chemical Physics</i> , 2005 , 122, 124508	3.9	106
113	Correlation Energy Expressions from the Adiabatic-Connection Fluctuation-Dissipation Theorem Approach. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 3116-30	6.4	103
112	Range-separated density-functional theory with the random-phase approximation: Detailed formalism and illustrative applications. <i>Physical Review A</i> , 2010 , 82,	2.6	103
111	Range separated hybrid density functional with long-range Hartree-Fock exchange applied to solids. <i>Journal of Chemical Physics</i> , 2007 , 127, 054101	3.9	86
110	Monomolecular cracking of propane over acidic chabazite: An ab initio molecular dynamics and transition path sampling study. <i>Journal of Catalysis</i> , 2011 , 279, 220-228	7.3	85
109	Comparison of ab Initio Hartree-Fock and Kohn-Sham Orbitals in the Calculation of Atomic Charge, Bond Index, and Valence. <i>Journal of Physical Chemistry A</i> , 2000 , 104, 9953-9963	2.8	83
108	Closed-shell ring coupled cluster doubles theory with range separation applied on weak intermolecular interactions. <i>Journal of Chemical Physics</i> , 2011 , 135, 084119	3.9	81
107	The origin of the problems with the PM3 core repulsion function. <i>Computational and Theoretical Chemistry</i> , 1997 , 393, 31-38		80
106	Approximate electrostatic interaction operator for QM/MM calculations. <i>Chemical Physics Letters</i> , 2002 , 356, 331-339	2.5	79
105	Reaction field factors for a multipole distribution in a cavity surrounded by a continuum. <i>Chemical Physics Letters</i> , 1993 , 202, 18-22	2.5	78
104	Blind test of density-functional-based methods on intermolecular interaction energies. <i>Journal of Chemical Physics</i> , 2016 , 145, 124105	3.9	76
103	Choosing between alternative MP2 algorithms in the self-consistent reaction field theory of solvent effects. <i>Chemical Physics Letters</i> , 1995 , 241, 51-56	2.5	71
102	Effect of Polarizability on the Potential of Mean Force of Two Cations. The Guanidinium-Guanidinium Ion Pair in Water. <i>Journal of Physical Chemistry B</i> , 1997 , 101, 10910-10917	3.4	70
101	Many-body dispersion corrections for periodic systems: an efficient reciprocal space implementation. <i>Journal of Physics Condensed Matter</i> , 2016 , 28, 045201	1.8	69
100	On the equivalence of ring-coupled cluster and adiabatic connection fluctuation-dissipation theorem random phase approximation correlation energy expressions. <i>Journal of Chemical Physics</i> , 2010 , 133, 154106	3.9	67
99	Modeling spin-crossover compounds by periodic DFT+U approach. <i>Physical Review B</i> , 2008 , 78,	3.3	67
98	Distributed polarizability of the water dimer: Field-induced charge transfer along the hydrogen bond. <i>Journal of Chemical Physics</i> , 2001 , 114, 7951-7961	3.9	67
97	Transferable net atomic charges from a distributed multipole analysis for the description of electrostatic properties: a case study of saturated hydrocarbons. <i>The Journal of Physical Chemistry</i> , 1993 , 97, 6628-6636		67

96	Charge Density Analysis and Topological Properties of Hal3-Synthons and Their Comparison with Competing Hydrogen Bonds. <i>Crystal Growth and Design</i> , 2012 , 12, 5373-5386	3.5	65
95	Common theoretical framework for quantum chemical solvent effect theories. <i>Journal of Mathematical Chemistry</i> , 1992 , 10, 93-137	2.1	63
94	A Fractionally Ionic Approach to Polarizability and van der Waals Many-Body Dispersion Calculations. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 5920-5930	6.4	62
93	Covalent bond orders and atomic valences from correlated wavefunctions. <i>Chemical Physics Letters</i> , 1999 , 299, 1-8	2.5	53
92	Spin crossover transition of Fe(phen) ₂ (NCS) ₂ : periodic dispersion-corrected density-functional study. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 5389-96	3.6	51
91	Potential curves for alkaline-earth dimers by density functional theory with long-range correlation corrections. <i>Chemical Physics Letters</i> , 2005 , 416, 370-375	2.5	51
90	Distributed first and second order hyperpolarizabilities: An improved calculation of nonlinear optical susceptibilities of molecular crystals. <i>Journal of Chemical Physics</i> , 2000 , 112, 6161-6172	3.9	51
89	On the Nature of Water Interacting with Brønsted Acidic Sites. Ab Initio Molecular Dynamics Study of Hydrated HSAPO-34. <i>Journal of Physical Chemistry B</i> , 1998 , 102, 7307-7310	3.4	50
88	On the exchange-hole model of London dispersion forces. <i>Journal of Chemical Physics</i> , 2007 , 127, 024108.9	3.9	49
87	Proton exchange of small hydrocarbons over acidic chabazite: Ab initio study of entropic effects. <i>Journal of Catalysis</i> , 2007 , 250, 171-183	7.3	48
86	Quantum-chemical model calculations on the acidic site of zeolites including Madelung-potential effects. <i>Chemical Physics Letters</i> , 1990 , 168, 461-467	2.5	48
85	A comprehensive approach to molecular charge density models: From distributed multipoles to fitted atomic charges. <i>International Journal of Quantum Chemistry</i> , 1994 , 52, 17-37	2.1	45
84	Intermolecular interaction energies by topologically partitioned electric properties II. Dispersion energies in one-centre and multicentre multipole expansions. <i>Molecular Physics</i> , 1997 , 91, 145-160	1.7	43
83	Ab initio study of structure and interconversion of native cellulose phases. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 10097-105	2.8	38
82	Distributed polarizabilities derived from induction energies: A finite perturbation approach. <i>Journal of Chemical Physics</i> , 2000 , 112, 2709-2717	3.9	38
81	Periodic projector augmented wave density functional calculations on the hexachlorobenzene crystal and comparison with the experimental multipolar charge density model. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 14484-94	2.8	37
80	OPEP: a tool for the optimal partitioning of electric properties. <i>Journal of Computational Chemistry</i> , 2003 , 24, 997-1008	3.5	37
79	Electrostatic interactions in three-dimensional solids. Self-consistent Madelung potential (SCMP) approach. <i>Journal of Chemical Physics</i> , 1987 , 86, 6957-6966	3.9	36

78	Molecular electrostatic fields from bond fragments. <i>International Journal of Quantum Chemistry</i> , 1987 , 31, 927-939	2.1	36
77	Derivation of Distributed Models of Atomic Polarizability for Molecular Simulations. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 1901-13	6.4	35
76	Comparison of protein electrostatic potential along the catalytic triad of serine proteinases. <i>Journal of Theoretical Biology</i> , 1983 , 103, 349-56	2.3	35
75	Aurophilic Interactions from Wave Function, Symmetry-Adapted Perturbation Theory, and Rangehybrid Approaches. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 2399-407	6.4	34
74	Rayleigh-Schrödinger perturbation theory for nonlinear Schrödinger equations with linear perturbation. <i>International Journal of Quantum Chemistry</i> , 1993 , 47, 469-483	2.1	34
73	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. <i>Journal De Chimie Physique Et De Physico-Chimie Biologique</i> , 1990 , 67, 875-888		34
72	Spin-unrestricted random-phase approximation with range separation: Benchmark on atomization energies and reaction barrier heights. <i>Journal of Chemical Physics</i> , 2015 , 142, 154123	3.9	33
71	Modeling Induction Phenomena in Intermolecular Interactions with an Ab Initio Force Field. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 1914-26	6.4	33
70	A SCRF-CNDO/2 study on proton conductivity mechanisms in hydronium perchlorate. Towards a quantum chemical representation of defects and impurities in crystals. <i>Journal of Chemical Physics</i> , 1982 , 77, 4723-4733	3.9	32
69	Intermolecular interaction energies by topologically partitioned electric properties. 1. Electrostatic and induction energies in one-centre and multicentre multipole expansions. <i>Molecular Physics</i> , 1996 , 88, 69-92	1.7	32
68	Statistical analysis of distributed multipoles derived from molecular electrostatic potentials. <i>Molecular Physics</i> , 1998 , 94, 881-895	1.7	31
67	Fast and accurate determination of induction energies: reduction of topologically distributed polarizability models. <i>Chemical Physics Letters</i> , 2001 , 338, 180-188	2.5	30
66	Crystal and electronic structure of two polymorphic modifications of famotidine. An experimental and theoretical study. <i>Computational and Theoretical Chemistry</i> , 2000 , 503, 73-79		30
65	Perturbation theory for nonlinear time-independent Schrödinger equations. <i>Physical Review A</i> , 1983 , 28, 45-48	2.6	30
64	Short range DFT combined with long-range local RPA within a range-separated hybrid DFT framework. <i>Chemical Physics Letters</i> , 2012 , 550, 162-169	2.5	28
63	Modeling amino acid side chains. 2. Determination of point charges from electrostatic properties: toward transferable point charge models. <i>The Journal of Physical Chemistry</i> , 1993 , 97, 9788-9796		28
62	Critical analysis of electric field modeling: Formamide. <i>Journal of Computational Chemistry</i> , 1992 , 13, 1234-1245	3.5	28
61	Dielectric Matrix Formulation of Correlation Energies in the Random Phase Approximation: Inclusion of Exchange Effects. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 2191-202	6.4	27

60	Transferability of topologically partitioned polarizabilities: the case of n-alkanes. <i>Molecular Physics</i> , 1996 , 89, 595-605	1.7	27
59	Linear scaling algorithm for the coordinate transformation problem of molecular geometry optimization. <i>Journal of Chemical Physics</i> , 2000 , 113, 5598-5603	3.9	26
58	Ab initio and DFT investigations of intramolecular hydrogen bonding in 1,2-ethanediol. <i>Chemical Physics Letters</i> , 1995 , 245, 129-135	2.5	26
57	Dispersion interaction in hydrogen-chain models. <i>Journal of Chemical Physics</i> , 2011 , 134, 114106	3.9	24
56	Alternative Approaches for the Calculation of Induction Energies: Characterization, Effectiveness, and Pitfalls. <i>Journal of Physical Chemistry A</i> , 2001 , 105, 11505-11514	2.8	23
55	Topologically partitioned dynamic polarizabilities using the theory of atoms in molecules. <i>Canadian Journal of Chemistry</i> , 1996 , 74, 976-987	0.9	23
54	Rayleigh-Schrödinger many-body perturbation theory for density functionals: A unified treatment of one- and two-electron perturbations. <i>Physical Review A</i> , 2008 , 78,	2.6	22
53	Intramolecular sulfur-oxygen interaction: An ab initio conformational study of (Z)-3-fluorothio-2-propenal. <i>Computational and Theoretical Chemistry</i> , 1985 , 123, 189-201		22
52	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. <i>Journal of the American Chemical Society</i> , 1986 , 108, 1275-1281	16.4	22
51	Mixed quantumclassical calculations on the water molecule in liquid phase: Influence of a polarizable environment on electronic properties. <i>International Journal of Quantum Chemistry</i> , 1996 , 58, 251-265	2.1	21
50	Analytical first and second energy derivatives in the polarization model. <i>Chemical Physics Letters</i> , 1990 , 166, 180-188	2.5	21
49	The Black Polymorph of TTF-CA: TTF Polymorphism and Solvent Effects in Mechanochemical and Vapor Digestion Syntheses, FT-IR, Crystal Packing, and Electronic Structure. <i>Crystal Growth and Design</i> , 2014 , 14, 91-100	3.5	20
48	Determination of Distributed Polarizabilities from a Statistical Analysis of Induction Energies. <i>Journal of Physical Chemistry A</i> , 2000 , 104, 1293-1303	2.8	20
47	Performance of Cu ⁺ , Pb ⁺ , and Hg ⁺ -Exchanged Mordenite in the Adsorption of I ₂ , ICH ₃ , H ₂ O, CO, ClCH ₃ , and Cl ₂ : A Density Functional Study. <i>ChemPhysChem</i> , 2017 , 18, 1642-1652	3.2	19
46	Analytical Energy Gradients in Range-Separated Hybrid Density Functional Theory with Random Phase Approximation. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 1968-79	6.4	19
45	The reliability of the point charge model representing intermolecular effects in ab initio calculations. <i>Chemical Physics Letters</i> , 1994 , 225, 258-264	2.5	19
44	A study on the backbone/side-chain interaction in N-formyl-(L)serineamide. <i>Canadian Journal of Chemistry</i> , 1990 , 68, 1882-1888	0.9	19
43	Continuing challenges in the parametrization of intermolecular force fields. Towards an accurate description of electrostatic and induction terms. <i>New Journal of Chemistry</i> , 2005 , 29, 411-420	3.6	18

42	Modeling amino acid side chains. 3. Influence of intra- and intermolecular environment on point charges. <i>The Journal of Physical Chemistry</i> , 1993 , 97, 9797-9807		18
41	Are direct reaction field methods appropriate for describing dispersion interactions?. <i>Chemical Physics Letters</i> , 1990 , 175, 313-318	2.5	18
40	Assessment of range-separated time-dependent density-functional theory for calculating C6 dispersion coefficients. <i>Journal of Chemical Physics</i> , 2013 , 138, 194106	3.9	17
39	An efficient method for the coordinate transformation problem of massively three-dimensional networks. <i>Journal of Chemical Physics</i> , 2001 , 114, 9747-9753	3.9	17
38	The use of theoretical indices for the characterization of S?O linkage multiplicity. <i>Computational and Theoretical Chemistry</i> , 1988 , 165, 273-287		17
37	Linear Response and Measures of Electron Delocalization in Molecules. <i>Current Organic Chemistry</i> , 2011 , 15, 3609-3618	1.7	16
36	Modelling the electric field of water obtained from accurate SCF wave functions. <i>Chemical Physics Letters</i> , 1990 , 172, 55-61	2.5	16
35	Improving the accuracy of ground-state correlation energies within a plane-wave basis set: The electron-hole exchange kernel. <i>Journal of Chemical Physics</i> , 2016 , 145, 104105	3.9	15
34	Charge density reconstitution from approximate exchange-correlation holes. <i>Canadian Journal of Chemistry</i> , 2009 , 87, 1444-1450	0.9	14
33	Comment on New strategies to incorporate the solvent polarization in self-consistent reaction field and free-energy perturbation simulations[J. Chem. Phys. 103, 10183 (1995)]. <i>Journal of Chemical Physics</i> , 1997 , 107, 1291-1292	3.9	14
32	OSIPE is a tool for scientific programming in FORTRAN. <i>Computer Physics Communications</i> , 1994 , 81, 293-317	4.2	14
31	Intermolecular Interaction Energies from Experimental Charge Density Studies 2011 , 387-433		13
30	Colour Polymorphism of a Bis(quinoline) Compound. <i>European Journal of Organic Chemistry</i> , 1999 , 1999, 2119-2125	3.2	13
29	Surface modification by substitution. <i>Chemical Physics Letters</i> , 1987 , 136, 1-8	2.5	13
28	Spherical harmonic expansion of short-range screened Coulomb interactions. <i>Journal of Physics A</i> , 2006 , 39, 8613-8630		12
27	Normalization corrections to perturbation theory for the time-independent nonlinear Schrödinger equation. <i>Physical Review A</i> , 1991 , 44, 2188-2191	2.6	12
26	Bond orders in three-centre bonds. <i>Computational and Theoretical Chemistry</i> , 1989 , 186, 61-67		12
25	Wigner's (2n + 1) rule for nonlinear Schrödinger equations. <i>Journal of Mathematical Chemistry</i> , 2009 , 46, 1-14	2.1	11

24	Intra- and intermolecular interactions in crystals of polar molecules. A study by the mixed quantum mechanical/molecular mechanical SCMP-NDDO method. <i>Journal of Computational Chemistry</i> , 2001 , 22, 1679-1690	3.5	11
23	Theoretical CD spectrum calculations of the crown-ether aralkyl-ammonium salt complex. <i>Chirality</i> , 2002 , 14, 377-85	2.1	10
22	Calculation of electrostatic potentials and fields inside zeolite cavities. <i>Collection of Czechoslovak Chemical Communications</i> , 1988 , 53, 2308-2319		9
21	Correlation of bond orders and softnesses. <i>Computational and Theoretical Chemistry</i> , 2000 , 501-502, 379-388		8
20	Calculations on electrostatic properties of HY zeolite. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1990 , 86, 3461-3466		8
19	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. <i>Theoretical Chemistry Accounts</i> , 2000 , 103, 238-241	1.9	7
18	Casimir-Polder Size Consistency: A Constraint Violated by Some Dispersion Theories. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 5829-5833	6.4	6
17	Ab initio determination of electronic energy splitting and transition rates for imidogen in argon matrixes. <i>The Journal of Physical Chemistry</i> , 1993 , 97, 10011-10020		6
16	The role of optimum supplementary d-orbitals for hypervalent selenium compounds. <i>Chemical Physics Letters</i> , 1986 , 131, 247-251	2.5	6
15	Electrostatic complementarity in molecular aggregates. <i>Computational and Theoretical Chemistry</i> , 1987 , 149, 169-176		6
14	Chemical Fragmentation Approach to the Quantum Chemical Description of Extended Systems 1991 , 1-49		6
13	Assessment of a range-separated orbital-optimised random-phase approximation electron correlation method. <i>Theoretical Chemistry Accounts</i> , 2018 , 137, 1	1.9	6
12	The role of induction forces in infra-red matrix shifts: quantum chemical calculations with reaction field model hamiltonian. <i>Computational and Theoretical Chemistry</i> , 1991 , 232, 97-110		5
11	Protein electrostatics on personal computers. <i>Computational and Theoretical Chemistry</i> , 1992 , 256, 113-123		5
10	Relationships between charge density response functions, exchange holes and localized orbitals. <i>Computational and Theoretical Chemistry</i> , 2015 , 1053, 44-52	2	4
9	Intramolecular sulfur-oxygen interaction in sulfonium compounds and sulfoxides. <i>Computational and Theoretical Chemistry</i> , 1989 , 186, 53-60		4
8	Computational chemistry on a PC. <i>International Journal of Quantum Chemistry</i> , 1990 , 38, 163-171	2.1	3
7	Synthesis of Vinca alkaloids and related compounds. Part 18. Stereochemical investigations on some intermediates leading to (+)-vincamine. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1984 , 1629-1636		3

6	Structure and ring inversion of 2-pyrrolidone. Semiempirical quantum chemical study and analysis of X-ray data. <i>Collection of Czechoslovak Chemical Communications</i> , 1986 , 51, 249-263		3
5	Ab Initio Simulations of Zeolite Reactivity. <i>Progress in Theoretical Chemistry and Physics</i> , 2001 , 77-108	0.6	3
4	Local random phase approximation with projected oscillator orbitals. <i>Theoretical Chemistry Accounts</i> , 2015 , 134, 1	1.9	2
3	Ab initio quantum chemical study of the structure and vibrational spectra of the vinylene carbonate molecule. <i>The Journal of Physical Chemistry</i> , 1986 , 90, 6420-6424		2
2	Chemical Fragmentation Approach to the Quantum Chemical Description of Extended Systems 1991 , 1-49		2
1	Spooky correlations and unusual van der Waals forces between gapless and near-gapless molecules. <i>Journal of Chemical Physics</i> , 2016 , 145, 204107	3.9	2