Jan Å˜ezÃ¡Ä•

List of Publications by Year
in descending order

109 papers	9,125 citations	57681 46 h-index	45040 94 g-index
125 all docs	125 docs citations	125 times ranked	7974 citing authors

#	Article	IF	Citations
1	Spin-component-scaled and dispersion-corrected second-order MÃ¸llerâ€“Plesset perturbation theory: a path toward chemical accuracy. Physical Chemistry Chemical Physics, 2022, 24, 3695-3712.	1.3	13
2	Non-Covalent Interactions Atlas benchmark data sets 5: London dispersion in an extended chemical space. Physical Chemistry Chemical Physics, 2022, 24, 14780-14793.	1.3	26
3	Non-covalent interactions atlas benchmark data sets 4: Ïƒ-hole interactions. Physical Chemistry Chemical Physics, 2022, 24, 14794-14804.	1.3	27
4	Conformational energies and equilibria of cyclic dinucleotidesin vacuoand in solution: computational chemistryvs.NMR experiments. Physical Chemistry Chemical Physics, 2021, 23, 7280-7294.	1.3	5
5	Non-Covalent Interactions Atlas Benchmark Data Sets 3: Repulsive Contacts. Journal of Chemical Theory and Computation, 2021, 17, 1548-1561.	2.3	42
6	SQM/COSMO Scoring Function: Reliable Quantumâ€Mechanical Tool for Sampling and Ranking in Structureâ€Based Drug Design. ChemPlusChem, 2020, 85, 2361-2361.	1.3	4
7	Non-Covalent Interactions Atlas Benchmark Data Sets 2: Hydrogen Bonding in an Extended Chemical Space. Journal of Chemical Theory and Computation, 2020, 16, 6305-6316.	2.3	47
8	Benchmark Data Sets of Boron Cluster Dihydrogen Bonding for the Validation of Approximate Computational Methods. ChemPhysChem, 2020, 21, 2599-2604.	1.0	4
9	SQM/COSMO Scoring Function: Reliable Quantumâ€Mechanical Tool for Sampling and Ranking in Structureâ€Based Drug Design. ChemPlusChem, 2020, 85, 2362-2371.	1.3	12
10	Non-Covalent Interactions Atlas Benchmark Data Sets: Hydrogen Bonding. Journal of Chemical Theory and Computation, 2020, 16, 2355-2368.	2.3	63
11	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	1.2	589
12	Benchmarking of Semiempirical Quantum-Mechanical Methods on Systems Relevant to Computer-Aided Drug Design. Journal of Chemical Information and Modeling, 2020, 60, 1453-1460.	2.5	45
13	Impressive Enrichment of Semiempirical Quantum Mechanicsâ€Based Scoring Function: HSP90 Protein with 4541 Inhibitors and Decoys. ChemPhysChem, 2019, 20, 2721-2721.	1.0	3
14	Impressive Enrichment of Semiempirical Quantum Mechanicsâ€Based Scoring Function: HSP90 Protein with 4541 Inhibitors and Decoys. ChemPhysChem, 2019, 20, 2759-2766.	1.0	11
15	Description of halogen bonding in semiempirical quantumâ€mechanical and selfâ€consistent charge densityâ€functional tightâ€binding methods. Journal of Computational Chemistry, 2019, 40, 1633-1642.	1.5	7
16	Reparametrization of the COSMO Solvent Model for Semiempirical Methods PM6 and PM7. Journal of Chemical Information and Modeling, 2019, 59, 229-235.	2.5	36
17	Toward Accurate Conformational Energies of Smaller Peptides and Medium-Sized Macrocycles: MPCONF196 Benchmark Energy Data Set. Journal of Chemical Theory and Computation, 2018, 14, 1254-1266.	2.3	69
18	Testing Semiempirical Quantum Mechanical Methods on a Data Set of Interaction Energies Mapping Repulsive Contacts in Organic Molecules. Journal of Physical Chemistry A, 2018, 122, 2801-2808.	1.1	22

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19	Ranking Power of the SQM/COSMO Scoring Function on Carbonic Anhydraseâ€...Iiâ€“Inhibitor Complexes. ChemPhysChem, 2018, 19, 873-879.	1.0	29
20	Macrocycle Conformational Sampling by DFT-D3/COSMO-RS Methodology. Journal of Chemical Information and Modeling, 2018, 58, 48-60.	2.5	19
21	Gating the electron transfer at a monocopper centre through the supramolecular coordination of water molecules within a protein chamber mimic. Chemical Science, 2018, 9, 8282-8290.	3.7	8
22	Accurate Noncovalent Interactions via Dispersion-Corrected Second-Order MÃllerâ€“Plesset Perturbation Theory. Journal of Chemical Theory and Computation, 2018, 14, 4711-4721.	2.3	41
23	SQM/COSMO Scoring Function at the DFTB3-D3H4 Level: Unique Identification of Native Proteinâ€“Ligand Poses. Journal of Chemical Information and Modeling, 2017, 57, 127-132.	2.5	40
24	Description of nonâ€covalent interactions in SCCâ€DFTB methods. Journal of Computational Chemistry, 2017, 38, 688-697.	1.5	44
25	Empirical D3 Dispersion as a Replacement for ab Initio Dispersion Terms in Density Functional Theory-Based Symmetry-Adapted Perturbation Theory. Journal of Chemical Theory and Computation, 2017, 13, 1638-1646.	2.3	11
26	Bâ€“Hâ‹¯Ï€: a nonclassical hydrogen bond or dispersion contact?. Physical Chemistry Chemical Physics, 2017, 19, 18194-18200.	1.3	32
27	Pnictogen bonding in pyrazineâ€¢PnX5 (Pn = P, As, Sb and X = F, Cl, Br) complexes. Journal of Molecular Modeling, 2017, 23, 328.	0.8	18
28	Empirical Self-Consistent Correction for the Description of Hydrogen Bonds in DFTB3. Journal of Chemical Theory and Computation, 2017, 13, 4804-4817.	2.3	50
29	Accurate DFT-D3 Calculations in a Small Basis Set. Journal of Chemical Theory and Computation, 2017, 13, 3575-3585.	2.3	70
30	Superior Performance of the SQM/COSMO Scoring Functions in Native Pose Recognition of Diverse Proteinâ€“Ligand Complexes in Cognate Docking. ACS Omega, 2017, 2, 4022-4029.	1.6	22
31	Non-covalent interactions in anisoleâ€“(CO₂)_n (n = 1, 2) complexes. Physical Chemistry Chemical Physics, 2017, 19, 22749-22758.	1.3	3
32	On the role of charge transfer in halogen bonding. Physical Chemistry Chemical Physics, 2017, 19, 791-803.	1.3	85
33	Introduction: Noncovalent Interactions. Chemical Reviews, 2016, 116, 4911-4912.	23.0	116
34	Competition between Halogen, Hydrogen and Dihydrogen Bonding in Brominated Carboranes. ChemPhysChem, 2016, 17, 3373-3376.	1.0	40
35	A Nexus between Theory and Experiment: Nonâ€Empirical Quantum Mechanical Computational Methodology Applied to Cucurbit[n]urilâ‹...Guest Binding Interactions. Chemistry - A European Journal, 2016, 22, 17226-17238.	1.7	29
36	Cuby: An integrative framework for computational chemistry. Journal of Computational Chemistry, 2016, 37, 1230-1237.	1.5	131

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37	The SQM/COSMO filter: reliable native pose identification based on the quantum-mechanical description of proteinâ€“ligand interactions and implicit COSMO solvation. Chemical Communications, 2016, 52, 3312-3315.	2.2	55
38	Efficient Covalent Bond Formation in Gas-Phase Peptideâ€“Peptide Ion Complexes with the Photoleucine Stapler. Journal of the American Society for Mass Spectrometry, 2016, 27, 633-645.	1.2	18
39	Benchmark Calculations of Interaction Energies in Noncovalent Complexes and Their Applications. Chemical Reviews, 2016, 116, 5038-5071.	23.0	346
40	New Insight into the Nature of Bonding in the Dimers of Lappertâ€™s Stannylene and Its Ge Analogs: A Quantum Mechanical Study. Journal of Chemical Theory and Computation, 2016, 12, 1696-1704.	2.3	16
41	Binding Energies of the Ï€-Stacked Anisole Dimer: New Molecular Beam-Laser Spectroscopy Experiments and CCSD(T) Calculations. Chemistry - A European Journal, 2015, 21, 6637-6637.	1.7	3
42	QM/MM Calculations with deMon2k. Molecules, 2015, 20, 4780-4812.	1.7	20
43	Robust, Basis-Set Independent Method for the Evaluation of Charge-Transfer Energy in Noncovalent Complexes. Journal of Chemical Theory and Computation, 2015, 11, 528-537.	2.3	48
44	Binding Energies of the Ï€â€Stacked Anisole Dimer: New Molecular Beamâ€”Laser Spectroscopy Experiments and CCSD(T) Calculations. Chemistry - A European Journal, 2015, 21, 6740-6746.	1.7	18
45	Representative Amino Acid Side-Chain Interactions in Proteinâ€“DNA Complexes: A Comparison of Highly Accurate Correlated Ab Initio Quantum Mechanical Calculations and Efficient Approaches for Applications to Large Systems. Journal of Chemical Theory and Computation, 2015, 11, 4086-4092.	2.3	22
46	Benchmark Calculations of Three-Body Intermolecular Interactions and the Performance of Low-Cost Electronic Structure Methods. Journal of Chemical Theory and Computation, 2015, 11, 3065-3079.	2.3	87
47	Extensions and applications of the A24 data set of accurate interaction energies. Physical Chemistry Chemical Physics, 2015, 17, 19268-19277.	1.3	50
48	Structure and energetics of the anisoleâ€“Ar_n (n = 1, 2, 3) complexes: high-resolution resonant two-photon and threshold ionization experiments, and quantum chemical calculations. Physical Chemistry Chemical Physics, 2015, 17, 12530-12537.	1.3	8
49	The Effect of Halogen-to-Hydrogen Bond Substitution on Human Aldose Reductase Inhibition. ACS Chemical Biology, 2015, 10, 1637-1642.	1.6	45
50	Malonate-based inhibitors of mammalian serine racemase: Kinetic characterization and structure-based computational study. European Journal of Medicinal Chemistry, 2015, 89, 189-197.	2.6	49
51	Parameterization of the DFTB3 Method for Br, Ca, Cl, F, I, K, and Na in Organic and Biological Systems. Journal of Chemical Theory and Computation, 2015, 11, 332-342.	2.3	227
52	Evaluation of composite schemes for CCSDT(Q) calculations of interaction energies of noncovalent complexes. Physical Chemistry Chemical Physics, 2014, 16, 19115-19121.	1.3	15
53	Ab Initio Quantum Mechanical Description of Noncovalent Interactions at Its Limits: Approaching the Experimental Dissociation Energy of the HF Dimer. Journal of Chemical Theory and Computation, 2014, 10, 3066-3073.	2.3	39
54	Convergence of the Interaction Energies in Noncovalent Complexes in the Coupled-Cluster Methods Up to Full Configuration Interaction. Journal of Chemical Theory and Computation, 2013, 9, 3420-3428.	2.3	34

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55	Accuracy of Quantum Chemical Methods for Large Noncovalent Complexes. Journal of Chemical Theory and Computation, 2013, 9, 3364-3374.	2.3	275
56	Competition between halogen, dihalogen and hydrogen bonds in bromo- and iodomethanol dimers. Journal of Molecular Modeling, 2013, 19, 2879-2883.	0.8	18
57	Quantum Mechanical Scoring: Structural and Energetic Insights into Cyclin-Dependent Kinase 2 Inhibition by Pyrazolo[1,5-a]pyrimidines. Current Computer-Aided Drug Design, 2013, 9, 118-129.	0.8	5
58	Parallel low-memory quasi-Newton optimization algorithm for molecular structure. Chemical Physics Letters, 2013, 584, 10-13.	1.2	2
59	Investigation of the Hydroxylation Mechanism of Noncoupled Copper Oxygenases by Ab Initio Molecular Dynamics Simulations. Chemistry - A European Journal, 2013, 19, 17328-17337.	1.7	19
60	Quantum Mechanics-Based Scoring Rationalizes the Irreversible Inactivation of Parasitic Schistosoma mansoni Cysteine Peptidase by Vinyl Sulfone Inhibitors. Journal of Physical Chemistry B, 2013, 117, 14973-14982.	1.2	43
61	QM/MM Calculations Reveal the Different Nature of the Interaction of Two Carborane-Based Sulfamide Inhibitors of Human Carbonic Anhydrase II. Journal of Physical Chemistry B, 2013, 117, 16096-16104.	1.2	47
62	CCSD[T] Describes Noncovalent Interactions Better than the CCSD(T), CCSD(TQ), and CCSDT Methods. Journal of Chemical Theory and Computation, 2013, 9, 364-369.	2.3	68
63	Modulation of Aldose Reductase Inhibition by Halogen Bond Tuning. ACS Chemical Biology, 2013, 8, 2484-2492.	1.6	85
64	Basis Set Dependence of Interaction Energies Computed Using Composite Post-MP2 Methods. Journal of Chemical Theory and Computation, 2013, 9, 330-337.	2.3	12
65	The Semiempirical Quantum Mechanical Scoring Function for In Silico Drug Design. ChemPlusChem, 2013, 78, 921-931.	1.3	80
66	MP2.5 and MP2.X: Approaching CCSD(T) Quality Description of Noncovalent Interaction at the Cost of a Single CCSD Iteration. ChemPhysChem, 2013, 14, 698-707.	1.0	69
67	Describing Noncovalent Interactions beyond the Common Approximations: How Accurate Is the â€œGold Standard,â€•CCSD(T) at the Complete Basis Set Limit?. Journal of Chemical Theory and Computation, 2013, 9, 2151-2155.	2.3	365
68	On the performance of the semiempirical quantum mechanical PM6 and PM7 methods for noncovalent interactions. Chemical Physics Letters, 2013, 568-569, 161-166.	1.2	115
69	Halogen bond tunability II: the varying roles of electrostatic and dispersion contributions to attraction in halogen bonds. Journal of Molecular Modeling, 2013, 19, 4651-4659.	0.8	190
70	Quantum Mechanical Scoring: Structural and Energetic Insights into Cyclin-Dependent Kinase 2 Inhibition by Pyrazolo[1,5-a]pyrimidines. Current Computer-Aided Drug Design, 2013, 9, 118-129.	0.8	52
71	Advanced Corrections of Hydrogen Bonding and Dispersion for Semiempirical Quantum Mechanical Methods. Journal of Chemical Theory and Computation, 2012, 8, 141-151.	2.3	429
72	Assessment of the Performance of MP2 and MP2 Variants for the Treatment of Noncovalent Interactions. Journal of Physical Chemistry A, 2012, 116, 4159-4169.	1.1	107

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73	The performance of MP2.5 and MP2.X methods for nonequilibrium geometries of molecular complexes. Physical Chemistry Chemical Physics, 2012, 14, 13187.	1.3	20
74	New insights into the mechanism of electron transfer within flavohemoglobins: tunnelling pathways, packing density, thermodynamic and kinetic analyses. Physical Chemistry Chemical Physics, 2012, 14, 13872.	1.3	19
75	Benchmark Calculations of Noncovalent Interactions of Halogenated Molecules. Journal of Chemical Theory and Computation, 2012, 8, 4285-4292.	2.3	264
76	Robust and Efficient Constrained DFT Molecular Dynamics Approach for Biochemical Modeling. Journal of Chemical Theory and Computation, 2012, 8, 418-427.	2.3	51
77	Quantum effects in biological electron transfer. Physical Chemistry Chemical Physics, 2012, 14, 5902.	1.3	31
78	Evaluation of the performance of postâ€Hartreeâ€Fock methods in terms of intermolecular distance in noncovalent complexes. Journal of Computational Chemistry, 2012, 33, 691-694.	1.5	15
79	MP2.X: a generalized MP2.5 method that produces improved binding energies with smaller basis sets. Physical Chemistry Chemical Physics, 2011, 13, 21121.	1.3	41
80	Transmission Coefficients for Chemical Reactions with Multiple States: Role of Quantum Decoherence. Journal of the American Chemical Society, 2011, 133, 3883-3894.	6.6	22
81	Extrapolation and Scaling of the DFT-SAPT Interaction Energies toward the Basis Set Limit. Journal of Chemical Theory and Computation, 2011, 7, 685-689.	2.3	67
82	S66: A Well-balanced Database of Benchmark Interaction Energies Relevant to Biomolecular Structures. Journal of Chemical Theory and Computation, 2011, 7, 2427-2438.	2.3	821
83	Free-Energy Simulations of Hydrogen Bonding versus Stacking of Nucleobases on a Graphene Surface. Journal of Physical Chemistry C, 2011, 115, 19455-19462.	1.5	24
84	Extensions of the S66 Data Set: More Accurate Interaction Energies and Angular-Displaced Nonequilibrium Geometries. Journal of Chemical Theory and Computation, 2011, 7, 3466-3470.	2.3	201
85	On the reliability of the corrected semiempirical quantum chemical method (PM6-DH2) for assigning the protonation states in HIV-1 protease/inhibitor complexes. Collection of Czechoslovak Chemical Communications, 2011, 76, 457-479.	1.0	7
86	Semiempirical Quantum Mechanical Method PM6-DH2X Describes the Geometry and Energetics of CK2-Inhibitor Complexes Involving Halogen Bonds Well, While the Empirical Potential Fails. Journal of Physical Chemistry B, 2011, 115, 8581-8589.	1.2	80
87	Transferable scoring function based on semiempirical quantum mechanical PM6-DH2 method: CDK2 with 15 structurally diverse inhibitors. Journal of Computer-Aided Molecular Design, 2011, 25, 223-235.	1.3	48
88	Halogen bond tunability I: the effects of aromatic fluorine substitution on the strengths of halogen-bonding interactions involving chlorine, bromine, and iodine. Journal of Molecular Modeling, 2011, 17, 3309-3318.	0.8	374
89	A halogen-bonding correction for the semiempirical PM6 method. Chemical Physics Letters, 2011, 506, 286-289.	1.2	114
90	A Transferable H-Bonding Correction for Semiempirical Quantum-Chemical Methods. Journal of Chemical Theory and Computation, 2010, 6, 344-352.	2.3	249

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91	Stretched DNA Investigated Using Molecular-Dynamics and Quantum-Mechanical Calculations. Biophysical Journal, 2010, 98, 101-110.	0.2	19
92	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.	3.3	50
93	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.	2.3	58
94	A Reliable Docking/Scoring Scheme Based on the Semiempirical Quantum Mechanical PM6-DH2 Method Accurately Covering Dispersion and H-Bonding: HIV-1 Protease with 22 Ligands. Journal of Physical Chemistry B, 2010, 114, 12666-12678.	1.2	116
95	Spin-component scaled coupled-clusters singles and doubles optimized towards calculation of noncovalent interactions. Physical Chemistry Chemical Physics, 2010, 12, 9611.	1.3	63
96	Comparative Study of Selected Wave Function and Density Functional Methods for Noncovalent Interaction Energy Calculations Using the Extended S22 Data Set. Journal of Chemical Theory and Computation, 2010, 6, 2365-2376.	2.3	227
97	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.	2.3	312
98	Design of HIV Protease Inhibitors Based on Inorganic Polyhedral Metallacarboranes. Journal of Medicinal Chemistry, 2009, 52, 7132-7141.	2.9	132
99	Potentialâ€Energy and Freeâ€Energy Surfaces of Glycylâ€Phenylalanylâ€Alanine (GFA) Tripeptide: Experiment and Theory. Chemistry - A European Journal, 2008, 14, 4886-4898.	1.7	47
100	Benchmark database on isolated small peptides containing an aromatic side chain: comparison between wave function and density functional theory methods and empirical force field. Physical Chemistry Chemical Physics, 2008, 10, 2747.	1.3	146
101	Interpretation of Protein/Ligand Crystal Structure using QM/MM Calculations: Case of HIV-1 Protease/Metallacarborane Complex. Journal of Physical Chemistry B, 2008, 112, 15094-15102.	1.2	52
102	Benzene Dimer: High-Level Wave Function and Density Functional Theory Calculations. Journal of Chemical Theory and Computation, 2008, 4, 1829-1834.	2.3	232
103	Adsorption of Aromatic Hydrocarbons and Ozone at Environmental Aqueous Surfaces. Journal of Physical Chemistry A, 2008, 112, 4942-4950.	1.1	38
104	Benzene Dimer: Dynamic Structure and Thermodynamics Derived from On-the-Fly ab initio DFT-D Molecular Dynamic Simulations. Journal of Chemical Theory and Computation, 2008, 4, 1835-1840.	2.3	39
105	Quantum Chemical Benchmark Energy and Geometry Database for Molecular Clusters and Complex Molecular Systems (www.begdb.com): A Users Manual and Examples. Collection of Czechoslovak Chemical Communications, 2008, 73, 1261-1270.	1.0	144
106	Correlation Between the Thermodynamic Stability of DNA Duplexes and the Interaction and Solvation Energies of DNA Building Blocks. Collection of Czechoslovak Chemical Communications, 2008, 73, 161-174.	1.0	1
107	The Stabilization Energy of the GLU-LYS Salt Bridge in the Protein/Water Environment: Correlated Quantum Chemical ab initio, DFT and Empirical Potential Studies. Collection of Czechoslovak Chemical Communications, 2008, 73, 921-936.	1.0	2
108	Density-Functional, Density-Functional Tight-Binding, and Wave Function Calculations on Biomolecular Systemsâ€. Journal of Physical Chemistry A, 2007, 111, 5642-5647.	1.1	27

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109	On the Nature of DNA-Duplex Stability. Chemistry - A European Journal, 2007, 13, 2983-2989.	1.7	28