Jan Å˜ezÃ¡Ä•

List of Publications by Year
in descending order

109 papers	9,125 citations	50276 46 h-index	39675 94 g-index
125 all docs	125 docs citations	125 times ranked	7134 citing authors

#	Article	IF	Citations
1	S66: A Well-balanced Database of Benchmark Interaction Energies Relevant to Biomolecular Structures. Journal of Chemical Theory and Computation, 2011, 7, 2427-2438.	5.3	821
2	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	3.0	589
3	Advanced Corrections of Hydrogen Bonding and Dispersion for Semiempirical Quantum Mechanical Methods. Journal of Chemical Theory and Computation, 2012, 8, 141-151.	5.3	429
4	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.	1.8	374
5	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.	5.3	365
6	Benchmark Calculations of Interaction Energies in Noncovalent Complexes and Their Applications. Chemical Reviews, 2016, 116, 5038-5071.	47.7	346
7	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.	5.3	312
8	Accuracy of Quantum Chemical Methods for Large Noncovalent Complexes. Journal of Chemical Theory and Computation, 2013, 9, 3364-3374.	5.3	275
9	Benchmark Calculations of Noncovalent Interactions of Halogenated Molecules. Journal of Chemical Theory and Computation, 2012, 8, 4285-4292.	5.3	264
10	A Transferable H-Bonding Correction for Semiempirical Quantum-Chemical Methods. Journal of Chemical Theory and Computation, 2010, 6, 344-352.	5.3	249
11	Benzene Dimer: High-Level Wave Function and Density Functional Theory Calculations. Journal of Chemical Theory and Computation, 2008, 4, 1829-1834.	5.3	232
12	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.	5.3	227
13	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.	5.3	227
14	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.	5.3	201
15	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.	1.8	190
16	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.	2.8	146
17	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
18	Design of HIV Protease Inhibitors Based on Inorganic Polyhedral Metallacarboranes. Journal of Medicinal Chemistry, 2009, 52, 7132-7141.	6.4	132

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19	Cuby: An integrative framework for computational chemistry. Journal of Computational Chemistry, 2016, 37, 1230-1237.	3.3	131
20	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.	2.6	116
21	Introduction: Noncovalent Interactions. Chemical Reviews, 2016, 116, 4911-4912.	47.7	116
22	On the performance of the semiempirical quantum mechanical PM6 and PM7 methods for noncovalent interactions. Chemical Physics Letters, 2013, 568-569, 161-166.	2.6	115
23	A halogen-bonding correction for the semiempirical PM6 method. Chemical Physics Letters, 2011, 506, 286-289.	2.6	114
24	Assessment of the Performance of MP2 and MP2 Variants for the Treatment of Noncovalent Interactions. Journal of Physical Chemistry A, 2012, 116, 4159-4169.	2.5	107
25	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.	5.3	87
26	Modulation of Aldose Reductase Inhibition by Halogen Bond Tuning. ACS Chemical Biology, 2013, 8, 2484-2492.	3.4	85
27	On the role of charge transfer in halogen bonding. Physical Chemistry Chemical Physics, 2017, 19, 791-803.	2.8	85
28	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.	2.6	80
29	The Semiempirical Quantum Mechanical Scoring Function for In Silico Drug Design. ChemPlusChem, 2013, 78, 921-931.	2.8	80
30	Accurate DFT-D3 Calculations in a Small Basis Set. Journal of Chemical Theory and Computation, 2017, 13, 3575-3585.	5.3	70
31	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.	2.1	69
32	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.	5.3	69
33	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.	5.3	68
34	Extrapolation and Scaling of the DFT-SAPT Interaction Energies toward the Basis Set Limit. Journal of Chemical Theory and Computation, 2011, 7, 685-689.	5.3	67
35	Spin-component scaled coupled-clusters singles and doubles optimized towards calculation of noncovalent interactions. Physical Chemistry Chemical Physics, 2010, 12, 9611.	2.8	63
36	Non-Covalent Interactions Atlas Benchmark Data Sets: Hydrogen Bonding. Journal of Chemical Theory and Computation, 2020, 16, 2355-2368.	5.3	63

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37	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.	5.3	58
38	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.	4.1	55
39	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.	2.6	52
40	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.	1.2	52
41	Robust and Efficient Constrained DFT Molecular Dynamics Approach for Biochemical Modeling. Journal of Chemical Theory and Computation, 2012, 8, 418-427.	5.3	51
42	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.	7.1	50
43	Extensions and applications of the A24 data set of accurate interaction energies. Physical Chemistry Chemical Physics, 2015, 17, 19268-19277.	2.8	50
44	Empirical Self-Consistent Correction for the Description of Hydrogen Bonds in DFTB3. Journal of Chemical Theory and Computation, 2017, 13, 4804-4817.	5.3	50
45	Malonate-based inhibitors of mammalian serine racemase: Kinetic characterization and structure-based computational study. European Journal of Medicinal Chemistry, 2015, 89, 189-197.	5.5	49
46	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.	2.9	48
47	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.	5.3	48
48	Potentialâ€Energy and Freeâ€Energy Surfaces of Glycylâ€Phenylalanylâ€Alanine (GFA) Tripeptide: Experiment and Theory. Chemistry - A European Journal, 2008, 14, 4886-4898.	3.3	47
49	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.	2.6	47
50	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.	5.3	47
51	The Effect of Halogen-to-Hydrogen Bond Substitution on Human Aldose Reductase Inhibition. ACS Chemical Biology, 2015, 10, 1637-1642.	3.4	45
52	Benchmarking of Semiempirical Quantum-Mechanical Methods on Systems Relevant to Computer-Aided Drug Design. Journal of Chemical Information and Modeling, 2020, 60, 1453-1460.	5.4	45
53	Description of nonâ€covalent interactions in SCCâ€DFTB methods. Journal of Computational Chemistry, 2017, 38, 688-697.	3.3	44
54	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.	2.6	43

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55	Non-Covalent Interactions Atlas Benchmark Data Sets 3: Repulsive Contacts. Journal of Chemical Theory and Computation, 2021, 17, 1548-1561.	5.3	42
56	MP2.X: a generalized MP2.5 method that produces improved binding energies with smaller basis sets. Physical Chemistry Chemical Physics, 2011, 13, 21121.	2.8	41
57	Accurate Noncovalent Interactions via Dispersion-Corrected Second-Order MÃ¸llerâ€“Plesset Perturbation Theory. Journal of Chemical Theory and Computation, 2018, 14, 4711-4721.	5.3	41
58	Competition between Halogen, Hydrogen and Dihydrogen Bonding in Brominated Carboranes. ChemPhysChem, 2016, 17, 3373-3376.	2.1	40
59	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.	5.4	40
60	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.	5.3	39
61	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.	5.3	39
62	Adsorption of Aromatic Hydrocarbons and Ozone at Environmental Aqueous Surfaces. Journal of Physical Chemistry A, 2008, 112, 4942-4950.	2.5	38
63	Reparametrization of the COSMO Solvent Model for Semiempirical Methods PM6 and PM7. Journal of Chemical Information and Modeling, 2019, 59, 229-235.	5.4	36
64	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.	5.3	34
65	Bâ€“Hâ‹¯Ï€: a nonclassical hydrogen bond or dispersion contact?. Physical Chemistry Chemical Physics, 2017, 19, 18194-18200.	2.8	32
66	Quantum effects in biological electron transfer. Physical Chemistry Chemical Physics, 2012, 14, 5902.	2.8	31
67	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.	3.3	29
68	Ranking Power of the SQM/COSMO Scoring Function on Carbonic Anhydraseâ€…IIâ€“Inhibitor Complexes. ChemPhysChem, 2018, 19, 873-879.	2.1	29
69	On the Nature of DNA-Duplex Stability. Chemistry - A European Journal, 2007, 13, 2983-2989.	3.3	28
70	Density-Functional, Density-Functional Tight-Binding, and Wave Function Calculations on Biomolecular Systemsâ€. Journal of Physical Chemistry A, 2007, 111, 5642-5647.	2.5	27
71	Non-covalent interactions atlas benchmark data sets 4: Ïƒ-hole interactions. Physical Chemistry Chemical Physics, 2022, 24, 14794-14804.	2.8	27
72	Non-Covalent Interactions Atlas benchmark data sets 5: London dispersion in an extended chemical space. Physical Chemistry Chemical Physics, 2022, 24, 14780-14793.	2.8	26

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73	Free-Energy Simulations of Hydrogen Bonding versus Stacking of Nucleobases on a Graphene Surface. Journal of Physical Chemistry C, 2011, 115, 19455-19462.	3.1	24
74	Transmission Coefficients for Chemical Reactions with Multiple States: Role of Quantum Decoherence. Journal of the American Chemical Society, 2011, 133, 3883-3894.	13.7	22
75	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.	5.3	22
76	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.	3.5	22
77	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.	2.5	22
78	The performance of MP2.5 and MP2.X methods for nonequilibrium geometries of molecular complexes. Physical Chemistry Chemical Physics, 2012, 14, 13187.	2.8	20
79	QM/MM Calculations with deMon2k. Molecules, 2015, 20, 4780-4812.	3.8	20
80	Stretched DNA Investigated Using Molecular-Dynamics and Quantum-Mechanical Calculations. Biophysical Journal, 2010, 98, 101-110.	0.5	19
81	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.	2.8	19
82	Investigation of the Hydroxylation Mechanism of Noncoupled Copper Oxygenases by Ab Initio Molecular Dynamics Simulations. Chemistry - A European Journal, 2013, 19, 17328-17337.	3.3	19
83	Macrocycle Conformational Sampling by DFT-D3/COSMO-RS Methodology. Journal of Chemical Information and Modeling, 2018, 58, 48-60.	5.4	19
84	Competition between halogen, dihalogen and hydrogen bonds in bromo- and iodomethanol dimers. Journal of Molecular Modeling, 2013, 19, 2879-2883.	1.8	18
85	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.	3.3	18
86	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.	2.8	18
87	Pnictogen bonding in pyrazineâ€¢PnX5 (Pn = P, As, Sb and X = F, Cl, Br) complexes. Journal of Molecular Modeling, 2017, 23, 328.	1.8	18
88	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.	5.3	16
89	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.	3.3	15
90	Evaluation of composite schemes for CCSDT(Q) calculations of interaction energies of noncovalent complexes. Physical Chemistry Chemical Physics, 2014, 16, 19115-19121.	2.8	15

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91	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.	2.8	13
92	Basis Set Dependence of Interaction Energies Computed Using Composite Post-MP2 Methods. Journal of Chemical Theory and Computation, 2013, 9, 330-337.	5.3	12
93	SQM/COSMO Scoring Function: Reliable Quantumâ€Mechanical Tool for Sampling and Ranking in Structureâ€Based Drug Design. ChemPlusChem, 2020, 85, 2362-2371.	2.8	12
94	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.	5.3	11
95	Impressive Enrichment of Semiempirical Quantum Mechanicsâ€Based Scoring Function: HSP90 Protein with 4541 Inhibitors and Decoys. ChemPhysChem, 2019, 20, 2759-2766.	2.1	11
96	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.	2.8	8
97	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.	7.4	8
98	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
99	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.	3.3	7
100	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.	1.2	5
101	Conformational energies and equilibria of cyclic dinucleotidesin vacuoand in solution: computational chemistryvs.NMR experiments. Physical Chemistry Chemical Physics, 2021, 23, 7280-7294.	2.8	5
102	SQM/COSMO Scoring Function: Reliable Quantumâ€Mechanical Tool for Sampling and Ranking in Structureâ€Based Drug Design. ChemPlusChem, 2020, 85, 2361-2361.	2.8	4
103	Benchmark Data Sets of Boron Cluster Dihydrogen Bonding for the Validation of Approximate Computational Methods. ChemPhysChem, 2020, 21, 2599-2604.	2.1	4
104	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.	3.3	3
105	Non-covalent interactions in anisoleâ€“(CO₂)_n (n = 1, 2) complexes. Physical Chemistry Chemical Physics, 2017, 19, 22749-22758.	2.8	3
106	Impressive Enrichment of Semiempirical Quantum Mechanicsâ€Based Scoring Function: HSP90 Protein with 4541 Inhibitors and Decoys. ChemPhysChem, 2019, 20, 2721-2721.	2.1	3
107	Parallel low-memory quasi-Newton optimization algorithm for molecular structure. Chemical Physics Letters, 2013, 584, 10-13.	2.6	2
108	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

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109	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