

Accuracy of Quantum Chemical Methods for Large Non

Journal of Chemical Theory and Computation

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Citation Report

#	ARTICLE	IF	CITATIONS
3	Off-Center Gaussian Functions, an Alternative Atomic Orbital Basis Set for Accurate Noncovalent Interaction Calculations of Large Systems. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5296-5304.	2.3	7
4	Efficient and accurate treatment of weak pairs in local CCSD(T) calculations. <i>Journal of Chemical Physics</i> , 2013, 139, 164116.	1.2	42
6	Contribution of phenylalanine side chain intercalation to the TATA-box binding proteinâ€™DNA interaction: molecular dynamics and dispersion-corrected density functional theory studies. <i>Journal of Molecular Modeling</i> , 2014, 20, 2499.	0.8	15
7	Shared memory multiprocessing implementation of resolution-of-the-identity second-order MÃ¶llerâ€™Plesset perturbation theory with attenuated and unattenuated results for intermolecular interactions between large molecules. <i>Molecular Physics</i> , 2014, 112, 836-843.	0.8	10
8	Low-Cost Quantum Chemical Methods for Noncovalent Interactions. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 4275-4284.	2.1	80
9	Studying Allosteric Regulation in Metal Sensor Proteins Using Computational Methods. <i>Advances in Protein Chemistry and Structural Biology</i> , 2014, 96, 181-218.	1.0	9
10	Approaching the complete basis set limit of CCSD(T) for large systems by the third-order incremental dual-basis set zero-buffer F12 method. <i>Journal of Chemical Physics</i> , 2014, 140, 044114.	1.2	12
11	Adsorption of Nitrogen-Containing Compounds on the (100) $\hat{\pm}$ -Quartz Surface: Ab Initio Cluster Approach. <i>Journal of Physical Chemistry C</i> , 2014, 118, 3023-3034.	1.5	17
12	Ab Initio Implementation of the Frenkelâ€™Davydov Exciton Model: A Naturally Parallelizable Approach to Computing Collective Excitations in Crystals and Aggregates. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5366-5376.	2.3	74
13	Theoretical study of adsorption of nitrogen-containing environmental contaminants on kaolinite surfaces. <i>Journal of Molecular Modeling</i> , 2014, 20, 2373.	0.8	9
14	Interaction Energy of Large Molecules from Restrained Denominator MP2-F12. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4857-4861.	2.3	12
15	Intermolecular interactions and charge transfer transitions in aromatic hydrocarbonâ€™tetracyanoethylene complexes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 20586-20597.	1.3	43
16	Selective induced polarization through electron transfer in acetone and pyrazole ester derivatives via Câ€™Hâ€™Oâ€™ interaction. <i>New Journal of Chemistry</i> , 2014, 38, 4885-4892.	1.4	10
17	ĩ%B97X-V: A 10-parameter, range-separated hybrid, generalized gradient approximation density functional with nonlocal correlation, designed by a survival-of-the-fittest strategy. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 9904.	1.3	616
18	Extending the applicability of the Tkatchenko-Scheffler dispersion correction via iterative Hirshfeld partitioning. <i>Journal of Chemical Physics</i> , 2014, 141, 034114.	1.2	174
19	Density functional tight binding: values of semi-empirical methods in an ab initio era. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14368-14377.	1.3	125
21	Optimization of the Coupled Cluster Implementation in NWChem on Petascale Parallel Architectures. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4307-4316.	2.3	31
22	Convergence of attenuated second order MÃ¶llerâ€™Plesset perturbation theory towards the complete basis set limit. <i>Chemical Physics Letters</i> , 2014, 608, 249-254.	1.2	5

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23	Wave Function and Density Functional Theory Studies of Dihydrogen Complexes. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3151-3162.	2.3	23
24	Quantum Mechanical Calculation of Noncovalent Interactions: A Large-Scale Evaluation of PMx, DFT, and SAPT Approaches. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1563-1575.	2.3	107
25	Separate Electronic Attenuation Allowing a Spin-Component-Scaled Second-Order Møller-Plesset Theory to Be Effective for Both Thermochemistry and Noncovalent Interactions. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6519-6525.	1.2	14
26	Investigation of topology of intermolecular interactions in the benzene-acetylene co-crystal by different theoretical methods. <i>Structural Chemistry</i> , 2014, 25, 1547-1552.	1.0	28
27	Accurate Modeling of Organic Molecular Crystals by Dispersion-Corrected Density Functional Tight Binding (DFTB). <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1785-1789.	2.1	155
28	Improving intermolecular interactions in DFTB3 using extended polarization from chemical-potential equalization. <i>Journal of Chemical Physics</i> , 2015, 143, 084123.	1.2	47
29	Benchmark calculations of the adsorption of aromatic molecules on graphene. <i>Journal of Computational Chemistry</i> , 2015, 36, 1763-1771.	1.5	23
30	Interplay between tetrel and triel bonds in $\text{RC}_6\text{H}_4\text{CN}^-\text{MF}_3^-\text{CN}^-\text{BX}_3^-$ complexes: A combined symmetry-adapted perturbation theory, Møller-Plesset, and quantum theory of atoms-in-molecules study. <i>Journal of Computational Chemistry</i> , 2015, 36, 2412-2428.	1.5	54
31	Quantum molecular modelling of ibuprofen bound to human serum albumin. <i>RSC Advances</i> , 2015, 5, 49439-49450.	1.7	42
32	Noncovalent Interactions of Heteroboranes. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2015, , 219-239.	0.6	4
34	The Nonlocal Correlation Density Functional VV10. <i>Annual Reports in Computational Chemistry</i> , 2015, 11, 37-102.	0.9	17
35	Determining the cohesive energy of coronene by dispersion-corrected DFT methods: Periodic boundary conditions vs. molecular pairs. <i>Journal of Chemical Physics</i> , 2015, 142, 054702.	1.2	10
36	Accurate Treatment of Large Supramolecular Complexes by Double-Hybrid Density Functionals Coupled with Nonlocal van der Waals Corrections. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 932-939.	2.3	48
37	Part and whole in wavefunction/DFT embedding. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	30
38	Benchmark Calculations of Three-Body Intermolecular Interactions and the Performance of Low-Cost Electronic Structure Methods. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3065-3079.	2.3	87
39	Theoretical description of 2D-cluster formation of nonionic surfactants at the air/water interface. <i>Colloid and Polymer Science</i> , 2015, 293, 3065-3089.	1.0	7
40	Comprehensive Benchmark of Association (Free) Energies of Realistic Host-Guest Complexes. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3785-3801.	2.3	188
41	Enhanced semiempirical QM methods for biomolecular interactions. <i>Computational and Structural Biotechnology Journal</i> , 2015, 13, 169-175.	1.9	61

#	ARTICLE	IF	CITATIONS
42	Mapping the genome of meta-generalized gradient approximation density functionals: The search for B97M-V. <i>Journal of Chemical Physics</i> , 2015, 142, 074111.	1.2	305
43	Nucleic acid reactivity: Challenges for next-generation semiempirical quantum models. <i>Journal of Computational Chemistry</i> , 2015, 36, 1370-1389.	1.5	14
44	Beyond Energies: Geometries of Nonbonded Molecular Complexes as Metrics for Assessing Electronic Structure Approaches. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1481-1492.	2.3	90
45	Consistent structures and interactions by density functional theory with small atomic orbital basis sets. <i>Journal of Chemical Physics</i> , 2015, 143, 054107.	1.2	605
46	Predicting Energetics of Supramolecular Systems Using the XDM Dispersion Model. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4033-4040.	2.3	39
47	Open challenges in structure-based virtual screening: Receptor modeling, target flexibility consideration and active site water molecules description. <i>Archives of Biochemistry and Biophysics</i> , 2015, 583, 105-119.	1.4	101
48	In silico studies on the origin of selective uptake of carbon dioxide with cucurbit[7]uril amorphous material. <i>RSC Advances</i> , 2015, 5, 72469-72475.	1.7	6
49	First-Principles Molecular Structure Search with a Genetic Algorithm. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 2338-2348.	2.5	83
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51	Toward Molecular Mechanism of Xenon Anesthesia: A Link to Studies of Xenon Complexes with Small Aromatic Molecules. <i>Journal of Physical Chemistry A</i> , 2015, 119, 2517-2521.	1.1	11
52	Parametrization of DFTB3/3OB for Magnesium and Zinc for Chemical and Biological Applications. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1062-1082.	1.2	138
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55	Comparison of one-parameter and linearly scaled one-parameter double-hybrid density functionals for noncovalent interactions. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1166-1172.	1.0	5
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60	Experimental and Theoretical Determination of Dissociation Energies of Dispersion-Dominated Aromatic Molecular Complexes. <i>Chemical Reviews</i> , 2016, 116, 5614-5641.	23.0	62
61	Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. <i>Chemical Reviews</i> , 2016, 116, 5301-5337.	23.0	312
62	Dispersion-Corrected Mean-Field Electronic Structure Methods. <i>Chemical Reviews</i> , 2016, 116, 5105-5154.	23.0	1,032
63	Accelerating Wave Function Convergence in Interactive Quantum Chemical Reactivity Studies. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1228-1235.	2.3	20
64	How Accurate is DFT for Iridium-Mediated Chemistry?. <i>Organometallics</i> , 2016, 35, 3795-3807.	1.1	76
65	A Nexus between Theory and Experiment: Non-Empirical Quantum Mechanical Computational Methodology Applied to Cucurbit[5]uril...Guest Binding Interactions. <i>Chemistry - A European Journal</i> , 2016, 22, 17226-17238.	1.7	29
66	Small Atomic Orbital Basis Set First-Principles Quantum Chemical Methods for Large Molecular and Periodic Systems: A Critical Analysis of Error Sources. <i>ChemistryOpen</i> , 2016, 5, 94-109.	0.9	57
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70	Cooperativity of intermolecular hydrogen bonds in microsolvated DMSO and DMF clusters: a DFT, AIM, and NCI analysis. <i>Journal of Molecular Modeling</i> , 2016, 22, 151.	0.8	40
71	Exchange-Correlation Effects for Noncovalent Interactions in Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3160-3175.	2.3	24
72	Vapor Liquid Equilibria of Hydrofluorocarbons Using Dispersion-Corrected and Nonlocal Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3295-3304.	2.3	11
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74	Functional molecules and materials by interaction based quantum theoretical design. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 622-633.	1.0	29
75	Modeling Polymorphic Molecular Crystals with Electronic Structure Theory. <i>Chemical Reviews</i> , 2016, 116, 5567-5613.	23.0	294
76	Benchmark Calculations of Interaction Energies in Noncovalent Complexes and Their Applications. <i>Chemical Reviews</i> , 2016, 116, 5038-5071.	23.0	346
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#	ARTICLE	IF	CITATIONS
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79	Structural Basis of the Interaction of Cyclin-Dependent Kinase...2 with Roscovitine and Its Analogues Having Bioisosteric Central Heterocycles. <i>ChemPhysChem</i> , 2017, 18, 785-795.	1.0	14
80	Conformational energy range of ligands in protein crystal structures: The difficult quest for accurate understanding. <i>Journal of Molecular Recognition</i> , 2017, 30, e2618.	1.1	23
81	First-Principles Models for van der Waals Interactions in Molecules and Materials: Concepts, Theory, and Applications. <i>Chemical Reviews</i> , 2017, 117, 4714-4758.	23.0	408
82	Host-guest interaction between tyrosine and β -cyclodextrin: Molecular modeling and nuclear studies. <i>Journal of Molecular Liquids</i> , 2017, 233, 358-363.	2.3	15
83	Quantum mechanical investigation of G-quartet systems of DNA. <i>New Journal of Chemistry</i> , 2017, 41, 2574-2585.	1.4	7
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85	Vanishing-Overhead Linear-Scaling Random Phase Approximation by Cholesky Decomposition and an Attenuated Coulomb-Metric. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1647-1655.	2.3	45
86	A Robust and Accurate Tight-Binding Quantum Chemical Method for Structures, Vibrational Frequencies, and Noncovalent Interactions of Large Molecular Systems Parametrized for All spd-Block Elements ($Z = 1-86$). <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1989-2009.	2.3	1,072
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89	Accuracy of finite-difference harmonic frequencies in density functional theory. <i>Journal of Computational Chemistry</i> , 2017, 38, 1678-1684.	1.5	14
90	Effect of dispersion corrections on covalent and non-covalent interactions in DFTB calculations. <i>Structural Chemistry</i> , 2017, 28, 1399-1407.	1.0	4
91	Improved Polarizable Dipole-Dipole Interaction Model for Hydrogen Bonding, Stacking, T-Shaped, and π - π Interactions. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2730-2741.	2.3	14
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#	ARTICLE	IF	CITATIONS
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98	Noncovalent Interactions in Specific Recognition Motifs of Protein-DNA Complexes. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 877-885.	2.3	22
99	Application of spin-ratio scaled MP2 for the prediction of intermolecular interactions in chemical systems. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 28936-28942.	1.3	21
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101	Benchmark Databases of Intermolecular Interaction Energies: Design, Construction, and Significance. <i>Annual Reports in Computational Chemistry</i> , 2017, 13, 3-91.	0.9	8
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103	A general intermolecular force field based on tight-binding quantum chemical calculations. <i>Journal of Chemical Physics</i> , 2017, 147, 161708.	1.2	53
104	Accurate DFT-D3 Calculations in a Small Basis Set. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3575-3585.	2.3	70
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110	Off-center Gaussian functions: Applications toward larger basis sets, post-second-order correlation treatment, and truncated virtual orbital space in investigations of noncovalent interactions. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25580.	1.0	3
111	Toward Accurate Conformational Energies of Smaller Peptides and Medium-Sized Macrocycles: MPCONF196 Benchmark Energy Data Set. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1254-1266.	2.3	69
112	Implications of monomer deformation for tetrel and pnictogen bonds. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8832-8841.	1.3	67
113	Accurate and Efficient Parallel Implementation of an Effective Linear-Scaling Direct Random Phase Approximation Method. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2505-2515.	2.3	35

#	ARTICLE	IF	CITATIONS
114	Atomic Orbital Implementation of Extended Symmetry-Adapted Perturbation Theory (XSAPT) and Benchmark Calculations for Large Supramolecular Complexes. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2955-2978.	2.3	43
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117	DFT Modeling of Cross-Linked Polyethylene: Role of Gold Atoms and Dispersion Interactions. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1496-1503.	1.1	8
118	Noncovalent interactions between cisplatin and graphene prototypes. <i>Journal of Computational Chemistry</i> , 2018, 39, 71-80.	1.5	13
119	S π -N chalcogen bonded complexes of carbon disulfide with diazines. Theoretical study. <i>Chemical Physics</i> , 2018, 500, 37-44.	0.9	12
120	Scalable Electron Correlation Methods. 5. Parallel Perturbative Triples Correction for Explicitly Correlated Local Coupled Cluster with Pair Natural Orbitals. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 198-215.	2.3	81
121	Computerchemie: das Schicksal aktueller Methoden und zukünftige Herausforderungen. <i>Angewandte Chemie</i> , 2018, 130, 4241-4248.	1.6	16
122	Computational Chemistry: The Fate of Current Methods and Future Challenges. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 4170-4176.	7.2	138
123	Low-scaling analytical gradients for the direct random phase approximation using an atomic orbital formalism. <i>Journal of Chemical Physics</i> , 2018, 149, 244111.	1.2	16
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#	ARTICLE	IF	CITATIONS
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134	Interaction between water and carbon nanostructures: How good are current density functional approximations?. <i>Journal of Chemical Physics</i> , 2019, 151, 164702.	1.2	47
135	Long-range dispersion-corrected density functional for noncovalent interactions. <i>International Journal of Modern Physics B</i> , 2019, 33, 1950300.	1.0	5
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137	Platinum, gold, and silver standards of intermolecular interaction energy calculations. <i>Journal of Chemical Physics</i> , 2019, 151, 070901.	1.2	33
138	HFLD: A Nonempirical London Dispersion-Corrected Hartree-Fock Method for the Quantification and Analysis of Noncovalent Interaction Energies of Large Molecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5894-5907.	2.3	36
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140	Physical adsorption of hydrogen molecules on single-walled carbon nanotubes and carbon-boron-nitrogen heteronanotubes: A comparative DFT study. <i>Vacuum</i> , 2019, 167, 280-286.	1.6	40
141	Theory and practice of modeling van der Waals interactions in electronic-structure calculations. <i>Chemical Society Reviews</i> , 2019, 48, 4118-4154.	18.7	114
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143	A generally applicable atomic-charge dependent London dispersion correction. <i>Journal of Chemical Physics</i> , 2019, 150, 154122.	1.2	697
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