

# 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.	5.3	7
4	Efficient and accurate treatment of weak pairs in local CCSD(T) calculations. <i>Journal of Chemical Physics</i> , 2013, 139, 164116.	3.0	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.	1.8	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.	1.7	10
8	Low-Cost Quantum Chemical Methods for Noncovalent Interactions. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 4275-4284.	4.6	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.	2.3	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.	3.0	12
11	Adsorption of Nitrogen-Containing Compounds on the (100) Î±-Quartz Surface: Ab Initio Cluster Approach. <i>Journal of Physical Chemistry C</i> , 2014, 118, 3023-3034.	3.1	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.	5.3	74
13	Theoretical study of adsorption of nitrogen-containing environmental contaminants on kaolinite surfaces. <i>Journal of Molecular Modeling</i> , 2014, 20, 2373.	1.8	9
14	Interaction Energy of Large Molecules from Restrained Denominator MP2-F12. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4857-4861.	5.3	12
15	Intermolecular interactions and charge transfer transitions in aromatic hydrocarbonâ€“tetracyanoethylene complexes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 20586-20597.	2.8	43
16	Selective induced polarization through electron transfer in acetone and pyrazole ester derivatives via Câ€“Hâ€“Oâ€“C interaction. <i>New Journal of Chemistry</i> , 2014, 38, 4885-4892.	2.8	10
17	Ï‰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.	2.8	616
18	Extending the applicability of the Tkatchenko-Scheffler dispersion correction via iterative Hirshfeld partitioning. <i>Journal of Chemical Physics</i> , 2014, 141, 034114.	3.0	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.	2.8	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.	5.3	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.	2.6	5

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24	Quantum Mechanical Calculation of Noncovalent Interactions: A Large-Scale Evaluation of PMx, DFT, and SAPT Approaches. Journal of Chemical Theory and Computation, 2014, 10, 1563-1575.	5.3	107
25	Separate Electronic Attenuation Allowing a Spin-Component-Scaled Second-Order Møller-Plesset Theory to Be Effective for Both Thermochemistry and Noncovalent Interactions. Journal of Physical Chemistry B, 2014, 118, 6519-6525.	2.6	14
26	Investigation of topology of intermolecular interactions in the benzene-acetylene co-crystal by different theoretical methods. Structural Chemistry, 2014, 25, 1547-1552.	2.0	28
27	Accurate Modeling of Organic Molecular Crystals by Dispersion-Corrected Density Functional Tight Binding (DFTB). Journal of Physical Chemistry Letters, 2014, 5, 1785-1789.	4.6	155
28	Improving intermolecular interactions in DFTB3 using extended polarization from chemical-potential equalization. Journal of Chemical Physics, 2015, 143, 084123.	3.0	47
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31	Quantum molecular modelling of ibuprofen bound to human serum albumin. RSC Advances, 2015, 5, 49439-49450.	3.6	42
32	Noncovalent Interactions of Heteroboranes. Challenges and Advances in Computational Chemistry and Physics, 2015, , 219-239.	0.6	4
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36	Accurate Treatment of Large Supramolecular Complexes by Double-Hybrid Density Functionals Coupled with Nonlocal van der Waals Corrections. Journal of Chemical Theory and Computation, 2015, 11, 932-939.	5.3	48
37	Part and whole in wavefunction/DFT embedding. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	30
38	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
39	Theoretical description of 2D-cluster formation of nonionic surfactants at the air/water interface. Colloid and Polymer Science, 2015, 293, 3065-3089.	2.1	7
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41	Enhanced semiempirical QM methods for biomolecular interactions. Computational and Structural Biotechnology Journal, 2015, 13, 169-175.	4.1	61

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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.	3.0	305
43	Nucleic acid reactivity: Challenges for next-generation semiempirical quantum models. <i>Journal of Computational Chemistry</i> , 2015, 36, 1370-1389.	3.3	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.	5.3	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.	3.0	605
46	Predicting Energetics of Supramolecular Systems Using the XDM Dispersion Model. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4033-4040.	5.3	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.	3.0	101
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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.	2.5	11
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53	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	1.7	2,561
54	Recent Progress in Treating Protein-Ligand Interactions with Quantum-Mechanical Methods. <i>International Journal of Molecular Sciences</i> , 2016, 17, 742.	4.1	29
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.	2.0	5
56	SparseMaps—A systematic infrastructure for reduced-scaling electronic structure methods. IV. Linear-scaling second-order explicitly correlated energy with pair natural orbitals. <i>Journal of Chemical Physics</i> , 2016, 144, 144109.	3.0	98
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61	Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. <i>Chemical Reviews</i> , 2016, 116, 5301-5337.	47.7	312
62	Dispersion-Corrected Mean-Field Electronic Structure Methods. <i>Chemical Reviews</i> , 2016, 116, 5105-5154.	47.7	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.	5.3	20
64	How Accurate is DFT for Iridium-Mediated Chemistry?. <i>Organometallics</i> , 2016, 35, 3795-3807.	2.3	76
65	A Nexus between Theory and Experiment: Non-Empirical Quantum Mechanical Computational Methodology Applied to Cucurbit[ <i>n</i> ]uril...Guest Binding Interactions. <i>Chemistry - A European Journal</i> , 2016, 22, 17226-17238.	3.3	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.	1.9	57
67	An Integral-Direct Linear-Scaling Second-Order Møller-Plesset Approach. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4897-4914.	5.3	72
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71	Exchange-Correlation Effects for Noncovalent Interactions in Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3160-3175.	5.3	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.	5.3	11
73	Cuby: An integrative framework for computational chemistry. <i>Journal of Computational Chemistry</i> , 2016, 37, 1230-1237.	3.3	131
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75	Modeling Polymorphic Molecular Crystals with Electronic Structure Theory. <i>Chemical Reviews</i> , 2016, 116, 5567-5613.	47.7	294
76	Benchmark Calculations of Interaction Energies in Noncovalent Complexes and Their Applications. <i>Chemical Reviews</i> , 2016, 116, 5038-5071.	47.7	346
77	Revealing the physical nature and the strength of charge-inverted hydrogen bonds by SAPT(DFT), MP2, SCS-MP2, MP2C, and CCSD(T) methods. <i>Journal of Computational Chemistry</i> , 2017, 38, 773-780.	3.3	17

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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.	2.1	14
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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.	47.7	408
82	Host-guest interaction between tyrosine and $\beta$ -cyclodextrin: Molecular modeling and nuclear studies. <i>Journal of Molecular Liquids</i> , 2017, 233, 358-363.	4.9	15
83	Quantum mechanical investigation of G-quartet systems of DNA. <i>New Journal of Chemistry</i> , 2017, 41, 2574-2585.	2.8	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.	5.3	45
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93	DSD-PBEP86-NL and DOD-PBEP86-NL functionals for noncovalent interactions: Basis set effects and tentative applications to large noncovalent systems. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25417.	2.0	6
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102	Scalable Electron Correlation Methods. 4. Parallel Explicitly Correlated Local Coupled Cluster with Pair Natural Orbitals (PNO-LCCSD-F12). <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4871-4896.	5.3	91
103	A general intermolecular force field based on tight-binding quantum chemical calculations. <i>Journal of Chemical Physics</i> , 2017, 147, 161708.	3.0	53
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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.	5.3	43
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118	Noncovalent interactions between cisplatin and graphene prototypes. <i>Journal of Computational Chemistry</i> , 2018, 39, 71-80.	3.3	13
119	S $\pi$ -N chalcogen bonded complexes of carbon disulfide with diazines. Theoretical study. <i>Chemical Physics</i> , 2018, 500, 37-44.	1.9	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.	5.3	81
121	Computerchemie: das Schicksal aktueller Methoden und zukünftige Herausforderungen. <i>Angewandte Chemie</i> , 2018, 130, 4241-4248.	2.0	16
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130	Extension of the atom by atom scheme of counterpoise method and presentation of its new advantages. <i>Journal of Chemical Physics</i> , 2018, 149, 064116.	3.0	2
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