Michal PitoÅˆÃ¡k

List of Publications by Year
in descending order

49 papers	4,997 citations	249298 26 h-index	242451 47 g-index
49 all docs	49 docs citations	49 times ranked	6001 citing authors

#	Article	IF	Citations
1	Machine learning prediction of 3CL SARS-CoV-2 docking scores. Computational Biology and Chemistry, 2022, 98, 107656.	1.1	9
2	Theoretical Study of the Monohydration of Mercury Compounds of Atmospheric Interest. Journal of Physical Chemistry A, 2021, 125, 5819-5828.	1.1	1
3	Assessment of scalar relativistic effects on halogen bonding and <scp>Ïƒâ€hole</scp> properties. International Journal of Quantum Chemistry, 2020, 120, e26392.	1.0	6
4	On the applicability of the MP2.5 approximation for open-shell systems. Case study of atmospheric reactivity. Computational and Theoretical Chemistry, 2020, 1186, 112901.	1.1	2
5	Offâ€center Gaussian functions: Applications toward larger basis sets, postâ€secondâ€order correlation treatment, and truncated virtual orbital space in investigations of noncovalent interactions. International Journal of Quantum Chemistry, 2018, 118, e25580.	1.0	3
6	Benchmark CCSD(T) and DFT study of binding energies in Be_{7 â^' 12}: in search of reliable DFT functional for beryllium clusters. Molecular Physics, 2018, 116, 1259-1274.	0.8	9
7	Adsorption of Organic Molecules to van der Waals Materials: Comparison of Fluorographene and Fluorographite with Graphene and Graphite. Journal of Chemical Theory and Computation, 2017, 13, 1328-1340.	2.3	47
8	Caesium hydride: MS-CASPT2 potential energy curves and A1Î£+â†'X1Î£+ absorption/emission spectroscopy. Journal of Chemical Physics, 2017, 146, 104304.	1.2	4
9	[Ni(bpy)(mal)(H2O)3]Â·H2O and [Ni(4,4â€²-dmbpy)(mal)(H2O)3]Â·1.5H2O: syntheses, crystal structures, magnetic properties, and computational study of stacking interactions. Journal of Coordination Chemistry, 2017, 70, 2999-3018.	0.8	9
10	Feâ€“Li Interactions in Ferrocenyllithium Compounds. European Journal of Inorganic Chemistry, 2017, 2017, 483-488.	1.0	3
11	Interactions of model biomolecules. Benchmark CC calculations within MOLCAS. , 2015, , .		0
12	Accuracy of Quantum Chemical Methods for Large Noncovalent Complexes. Journal of Chemical Theory and Computation, 2013, 9, 3364-3374.	2.3	275
13	Off-Center Gaussian Functions, an Alternative Atomic Orbital Basis Set for Accurate Noncovalent Interaction Calculations of Large Systems. Journal of Chemical Theory and Computation, 2013, 9, 5296-5304.	2.3	7
14	Ab initio study of many-body decomposition of the interaction energy in small beryllium clusters. Chemical Physics Letters, 2013, 573, 8-14.	1.2	13
15	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
16	Ab initiostudy of the stability of beryllium clusters: accurate calculations for Be_{2 â^' 6}. Journal of Physics B: Atomic, Molecular and Optical Physics, 2012, 45, 085102.	0.6	18
17	Highly correlated calculations using optimized virtual orbital space with controlled accuracy. Application to counterpoise corrected interaction energy calculations. International Journal of Quantum Chemistry, 2012, 112, 948-959.	1.0	9
18	Accuracy of Several Wave Function and Density Functional Theory Methods for Description of Noncovalent Interaction of Saturated and Unsaturated Hydrocarbon Dimers. Journal of Chemical Theory and Computation, 2012, 8, 2282-2292.	2.3	52

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19	Coupled Cluster and MÃ¸llerâ€“Plesset Perturbation Theory Calculations of Noncovalent Intermolecular Interactions using Density Fitting with Auxiliary Basis Sets from Cholesky Decompositions. Journal of Chemical Theory and Computation, 2012, 8, 1921-1928.	2.3	35
20	On the Structure and Geometry of Biomolecular Binding Motifs (Hydrogen-Bonding, Stacking, X-HÂ·Â·Â·Ï€): WFT and DFT Calculations. Journal of Chemical Theory and Computation, 2011, 7, 807-807.	2.3	3
21	Complete Basis Set Extrapolation and Hybrid Schemes for Geometry Gradients of Noncovalent Complexes. Journal of Chemical Theory and Computation, 2011, 7, 3924-3934.	2.3	24
22	Parallelized implementation of the CCSD(T) method in MOLCAS using optimized virtual orbitals space and Cholesky decomposed two-electron integrals. Collection of Czechoslovak Chemical Communications, 2011, 76, 713-742.	1.0	30
23	H-Bonding Cooperativity Effects in Amyloids: Quantum Mechanical and Molecular Mechanics Study. Zeitschrift Fur Physikalische Chemie, 2011, 225, 553-574.	1.4	7
24	On the Structure and Geometry of Biomolecular Binding Motifs (Hydrogen-Bonding, Stacking, Xâˆ’HÂ·Â·Â·Ï€): WFT and DFT Calculations. Journal of Chemical Theory and Computation, 2010, 6, 66-80.	2.3	175
25	A Transferable H-Bonding Correction for Semiempirical Quantum-Chemical Methods. Journal of Chemical Theory and Computation, 2010, 6, 344-352.	2.3	249
26	MOLCAS 7: The Next Generation. Journal of Computational Chemistry, 2010, 31, 224-247.	1.5	1,485
27	Stabilization and Structure Calculations for Noncovalent Interactions in Extended Molecular Systems Based on Wave Function and Density Functional Theories. Chemical Reviews, 2010, 110, 5023-5063.	23.0	697
28	Spin-component scaled coupled-clusters singles and doubles optimized towards calculation of noncovalent interactions. Physical Chemistry Chemical Physics, 2010, 12, 9611.	1.3	63
29	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
30	Three- and four-body nonadditivities in nucleic acid tetramers: a CCSD(T) study. Physical Chemistry Chemical Physics, 2010, 12, 1369-1378.	1.3	28
31	Accurate Intermolecular Interaction Energies from a Combination of MP2 and TDDFT Response Theory. Journal of Chemical Theory and Computation, 2010, 6, 168-178.	2.3	154
32	Coupled Cluster Calculations: Ovos as an Alternative Avenue Towards Treating Still Larger Molecules. Challenges and Advances in Computational Chemistry and Physics, 2010, , 429-454.	0.6	3
33	Scaled MP3 Nonâ€Covalent Interaction Energies Agree Closely with Accurate CCSD(T) Benchmark Data. ChemPhysChem, 2009, 10, 282-289.	1.0	232
34	CCSD(T) calculations of the electron affinity of the uracil molecule. Chemical Physics Letters, 2009, 481, 107-111.	1.2	19
35	Convergence of the CCSD(T) Correction Term for the Stacked Complex Methyl Adenineâˆ’Methyl Thymine: Comparison with Lower-Cost Alternatives. Journal of Chemical Theory and Computation, 2009, 5, 1761-1766.	2.3	55
36	Electron affinity of the O₂ molecule: CCSD(T) calculations using the optimized virtual orbitals space approach. International Journal of Quantum Chemistry, 2008, 108, 2159-2171.	1.0	37

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37	Highly Accurate CCSD(T) and DFTâ€“SAPT Stabilization Energies of Hâ€Bonded and Stacked Structures of the Uracil Dimer. ChemPhysChem, 2008, 9, 1636-1644.	1.0	110
38	Evaluation of the intramolecular basis set superposition error in the calculations of larger molecules: [n]helicenes and Pheâ€Glyâ€Phe tripeptide. Journal of Computational Chemistry, 2008, 29, 861-870.	1.5	64
39	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
40	Benzene Dimer: High-Level Wave Function and Density Functional Theory Calculations. Journal of Chemical Theory and Computation, 2008, 4, 1829-1834.	2.3	232
41	Toward More Efficient CCSD(T) Calculations of Intermolecular Interactions in Model Hydrogen-Bonded and Stacked Dimers. Journal of Physical Chemistry A, 2008, 112, 7115-7123.	1.1	23
42	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
43	CÏ£¿H Stretching Vibrational Shift of Benzene Dimer: Consistency of Experiment and Calculation. ChemPhysChem, 2007, 8, 2107-2111.	1.0	67
44	Optimized virtual orbitals for relativistic calculations: an alternative approach to the basis set construction for correlation calculations. Molecular Physics, 2006, 104, 2277-2292.	0.8	34
45	Optimized virtual orbitals for correlated calculations: Towards large scale CCSD(T) calculations of molecular dipole moments and polarizabilities. Computational and Theoretical Chemistry, 2006, 768, 79-89.	1.5	42
46	Optimized virtual orbital space (OVOS) as a tool for more efficient correlated and relativistic calculations of molecular properties and interactions. , 2006, , 265-285.		2
47	A study of H2Sâ€‰Â·Â·Â·â€‰NO+complex. Molecular Physics, 2005, 103, 2309-2319.	0.8	4
48	Optimized virtual orbitals for correlated calculations: an alternative approach. Molecular Physics, 2005, 103, 2141-2157.	0.8	62
49	Excited-state potential energy surfaces of silaethylene: a MRCI investigation. Molecular Physics, 2005, 103, 855-862.	0.8	8