Pavel Hobza

List of Publications by Year in descending order

546 papers	52,123 citations	1294 109 h-index	1792 211 g-index
576 all docs	576 docs citations	576 times ranked	28914 citing authors

#	Article	IF	Citations
1	The unusual stability of Hâ€bonded complexes in solvent caused by greater solvation energy of complex compared to those of isolated fragments. Journal of Computational Chemistry, 2023, 44, 329-333.	1.5	3
2	P-Doped grapheneâ€“C₆₀ nanocomposite: a donorâ€“acceptor complex with a Pâ€“C dative bond. Chemical Communications, 2022, 58, 1045-1048.	2.2	4
3	The stability of covalent dative bond significantly increases with increasing solvent polarity. Nature Communications, 2022, 13, 2107.	5.8	13
4	The Existence of a Nâ†'C Dative Bond in the C 60 â€“Piperidine Complex. Angewandte Chemie, 2021, 133, 1970-1978.	1.6	4
5	The Existence of a Nâ†'C Dative Bond in the C₆₀â€“Piperidine Complex. Angewandte Chemie - International Edition, 2021, 60, 1942-1950.	7.2	15
6	Multipodal insulin mimetics built on adamantane or proline scaffolds. Bioorganic Chemistry, 2021, 107, 104548.	2.0	3
7	Tuning the Pâ€“C dative/covalent bond formation in R₃Pâ€“C₆₀ complexes by changing the R group. Chemical Communications, 2021, 57, 3363-3366.	2.2	3
8	Structure-directed formation of the dative/covalent bonds in complexes with C₇₀â‹¯piperidine. Physical Chemistry Chemical Physics, 2021, 23, 4365-4375.	1.3	9
9	Cyclo[n]carbons Form Strong N â†' C Dative/Covalent Bonds with Piperidine. Journal of Physical Chemistry A, 2021, 125, 2923-2931.	1.1	13
10	The Structure-Based Design of SARS-CoV-2 nsp14 Methyltransferase Ligands Yields Nanomolar Inhibitors. ACS Infectious Diseases, 2021, 7, 2214-2220.	1.8	57
11	Addition Reaction between Piperidine and C₆₀ to Form 1,4-Disubstituted C₆₀ Proceeds through van der Waals and Dative Bond Complexes: Theoretical and Experimental Study. Journal of the American Chemical Society, 2021, 143, 10930-10939.	6.6	6
12	Azobenzene-Iron(III)porphyrin Hybrid Composite as a Light-Driven Molecular Spin Regulator: Some Promising Insights from DFT. Chemistry of Materials, 2021, 33, 8786-8799.	3.2	4
13	Real-space imaging of anisotropic charge of Ïƒ-hole by means of Kelvin probe force microscopy. Science, 2021, 374, 863-867.	6.0	71
14	Spin modification of iron(<scp>ii</scp>) complexes via covalent (dative) and dispersion guided non-covalent bonding with N-heterocyclic carbenes: DFT, DLPNO-CCSD(T) and MCSCF studies. Dalton Transactions, 2020, 49, 164-170.	1.6	5
15	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
16	Ground state of the Fe(<scp>ii</scp>)-porphyrin model system corresponds to quintet: a DFT and DMRG-based tailored CC study. Physical Chemistry Chemical Physics, 2020, 22, 17033-17037.	1.3	11
17	Directly linked metalloporphyrins: a quest for bio-inspired materials. Materials Advances, 2020, 1, 1895-1908.	2.6	4
18	ChelatingÂPolymers for Hereditary Hemochromatosis Treatment. Macromolecular Bioscience, 2020, 20, 2000254.	2.1	5

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19	Benchmark Data Sets of Boron Cluster Dihydrogen Bonding for the Validation of Approximate Computational Methods. ChemPhysChem, 2020, 21, 2599-2604.	1.0	4
20	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
21	Optimization of norbornylâ€based carbocyclic nucleoside analogs as cyclinâ€dependent kinase 2 inhibitors. Journal of Molecular Recognition, 2020, 33, e2842.	1.1	2
22	Mechanical force-induced manipulation of electronic conductance in a spin-crossover complex: a simple approach to molecular electronics. Nanoscale Advances, 2020, 2, 2907-2913.	2.2	11
23	Chalcogen Bonding due to the Exo-Substitution of Icosahedral Dicarbaborane. Molecules, 2019, 24, 2657.	1.7	6
24	Impressive Enrichment of Semiempirical Quantum Mechanicsâ€Based Scoring Function: HSP90 Protein with 4541 Inhibitors and Decoys. ChemPhysChem, 2019, 20, 2721-2721.	1.0	3
25	Impressive Enrichment of Semiempirical Quantum Mechanicsâ€Based Scoring Function: HSP90 Protein with 4541 Inhibitors and Decoys. ChemPhysChem, 2019, 20, 2759-2766.	1.0	11
26	Spin Crossover in Iron(II) Porphyrazine Induced by Noncovalent Interactions Combined with Hybridization of Iron(II) Porphyrazine and Ligandâ€™s Orbitals: CASPT2, CCSD(T), and DFT Studies. Journal of Physical Chemistry C, 2019, 123, 23186-23194.	1.5	5
27	Mutations at hypothetical binding site 2 in insulin and insulin-like growth factors 1 and 2 result in receptor- and hormone-specific responses. Journal of Biological Chemistry, 2019, 294, 17371-17382.	1.6	21
28	Structure and Properties of Double-Sandwich Complexes at the Graphene Surface: A Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 14712-14724.	1.5	4
29	Computational Approach To Understand the Adsorption Behavior of Iron(II) Phthalocyanine on the Doped Graphene Surface. Journal of Physical Chemistry C, 2019, 123, 6717-6724.	1.5	8
30	Nature of Binding in Planar Halogenâ€“Benzene Assemblies and Their Possible Visualization in Scanning Probe Microscopy. Journal of Physical Chemistry C, 2019, 123, 8379-8386.	1.5	6
31	Imidazo[1,2â€c]pyrimidinâ€5(6H)â€one as a novel core of cyclinâ€dependent kinase 2 inhibitors: Synthesis, activity measurement, docking, and quantum mechanical scoring. Journal of Molecular Recognition, 2018, 31, e2720.	1.1	10
32	Ranking Power of the SQM/COSMO Scoring Function on Carbonic Anhydraseâ€…IIâ€“Inhibitor Complexes. ChemPhysChem, 2018, 19, 873-879.	1.0	29
33	Various types of non-covalent interactions contributing towards crystal packing of halogenated diphospha-dicarbaborane with an open pentagonal belt. New Journal of Chemistry, 2018, 42, 10481-10483.	1.4	1
34	Sequential BN-doping induced tuning of electronic properties in zigzag-edged graphene nanoribbons: a computational approach. RSC Advances, 2018, 8, 10964-10974.	1.7	3
35	The role of the Ïƒ-holes in stability of non-bonded chalcogenideâ‹¯benzene interactions: the ground and excited states. Physical Chemistry Chemical Physics, 2018, 20, 299-306.	1.3	10
36	Sâ‹¯N chalcogen bonded complexes of carbon disulfide with diazines. Theoretical study. Chemical Physics, 2018, 500, 37-44.	0.9	12

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37	Understanding the non-covalent interaction mediated modulations on the electronic structure of quasi-zero-dimensional graphene nanoflakes. Physical Chemistry Chemical Physics, 2018, 20, 18718-18728.	1.3	2
38	Interface Interactions of the Bowmanâ€“Birk Inhibitor BTCI in a Ternary Complex with Trypsin and Chymotrypsin Evaluated by Semiempirical Quantum Mechanical Calculations. European Journal of Organic Chemistry, 2018, 2018, 5203-5211.	1.2	5
39	Non-covalent control of spin-state in metal-organic complex by positioning on N-doped graphene. Nature Communications, 2018, 9, 2831.	5.8	68
40	An Isolated Molecule of Iron(II) Phthalocyanin Exhibits Quintet Groundâ€State: A Nexus between Theory and Experiment. Chemistry - A European Journal, 2018, 24, 13413-13417.	1.7	12
41	Comparison of the DFT-SAPT and Canonical EDA Schemes for the Energy Decomposition of Various Types of Noncovalent Interactions. Journal of Chemical Theory and Computation, 2018, 14, 3440-3450.	2.3	74
42	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
43	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
44	Structural Basis of the Interaction of Cyclinâ€Dependent Kinaseâ€…2 with Roscovitine and Its Analogues Having Bioisosteric Central Heterocycles. ChemPhysChem, 2017, 18, 785-795.	1.0	14
45	Unraveling the Structureâ€“Affinity Relationship between Cucurbit[n]urils (n = 7, 8) and Cationic Diamondoids. Journal of the American Chemical Society, 2017, 139, 3249-3258.	6.6	66
46	Binary twinned-icosahedral [B₂₁H₁₈]^{â^’} interacts with cyclodextrins as a precedent for its complexation with other organic motifs. Physical Chemistry Chemical Physics, 2017, 19, 11748-11752.	1.3	26
47	Bâ€“Hâ‹¯Ï€: a nonclassical hydrogen bond or dispersion contact?. Physical Chemistry Chemical Physics, 2017, 19, 18194-18200.	1.3	32
48	Noncovalent Interactions in Specific Recognition Motifs of Proteinâ€“DNA Complexes. Journal of Chemical Theory and Computation, 2017, 13, 877-885.	2.3	22
49	Explicit treatment of active-site waters enhances quantum mechanical/implicit solvent scoring: Inhibition of CDK2 by new pyrazolo[1,5-a]pyrimidines. European Journal of Medicinal Chemistry, 2017, 126, 1118-1128.	2.6	32
50	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
51	Understanding the spin-dependent electronic properties of symmetrically far-edge doped zigzag graphene nanoribbon from a first principles study. RSC Advances, 2017, 7, 46604-46614.	1.7	10
52	Selective binding of choline by a phosphate-coordination-based triple helicate featuring an aromatic box. Nature Communications, 2017, 8, 938.	5.8	56
53	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
54	Non-covalent interactions in anisoleâ€“(CO₂)_n (n = 1, 2) complexes. Physical Chemistry Chemical Physics, 2017, 19, 22749-22758.	1.3	3

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55	The Interplay between Various Ïƒ- and Ï€-Hole Interactions of Trigonal Boron and Trigonal Pyramidal Arsenic Triiodides. Crystals, 2017, 7, 225.	1.0	6
56	IDD388 Polyhalogenated Derivatives as Probes for an Improved Structure-Based Selectivity of AKR1B10 Inhibitors. ACS Chemical Biology, 2016, 11, 2693-2705.	1.6	19
57	Experimental and Theoretical Study for the Assessment of the Conformational Stability of Polymethylene-Bridged Heteroaromatic Dimers: A Case of Unprecedented Folding. Crystal Growth and Design, 2016, 16, 1176-1180.	1.4	9
58	Introduction: Noncovalent Interactions. Chemical Reviews, 2016, 116, 4911-4912.	23.0	116
59	Competition between Halogen, Hydrogen and Dihydrogen Bonding in Brominated Carboranes. ChemPhysChem, 2016, 17, 3373-3376.	1.0	40
60	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
61	Ab initio and DFT studies of the interaction between carbonyl and thiocarbonyl groups: the role of SÂ·Â·Â·O chalcogen bonds. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	13
62	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
63	Computational methods for the description of pharmacologically relevant platinum complexes â€“ molecular structure and bond dissociation. Physical Chemistry Chemical Physics, 2016, 18, 4051-4062.	1.3	4
64	Computer Modeling of Halogen Bonds and Other Ïƒ-Hole Interactions. Chemical Reviews, 2016, 116, 5155-5187.	23.0	537
65	On the nature of the stabilisation of the Eâ‹¯Ï€ pnicogen bond in the SbCl₃â‹¯toluene complex. Chemical Communications, 2016, 52, 3500-3503.	2.2	39
66	Benchmark Calculations of Interaction Energies in Noncovalent Complexes and Their Applications. Chemical Reviews, 2016, 116, 5038-5071.	23.0	346
67	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
68	The non-planarity of the benzene molecule in the X-ray structure of the chelated bismuth(iii) heteroboroxine complex is not supported by quantum mechanical calculations. Dalton Transactions, 2016, 45, 462-465.	1.6	10
69	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
70	Halogen bonding origin properties and applications. AIP Conference Proceedings, 2015, , .	0.3	0
71	Interactions of model biomolecules. Benchmark CC calculations within MOLCAS. , 2015, , .		0
72	From Dibismuthenes to Threeâ€•and Twoâ€Coordinated Bismuthinidenes by Fine Ligand Tuning: Evidence for Aromatic BiC₃N Rings through a Combined Experimental and Theoretical Study. Chemistry - A European Journal, 2015, 21, 16917-16928.	1.7	76

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73	Noncovalent Interactions of Heteroboranes. Challenges and Advances in Computational Chemistry and Physics, 2015, , 219-239.	0.6	4
74	Chalcogen and Pnicogen Bonds in Complexes of Neutral Icosahedral and Bicapped Square-Antiprismatic Heteroboranes. Journal of Physical Chemistry A, 2015, 119, 1388-1395.	1.1	39
75	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
76	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
77	The properties of substituted 3D-aromatic neutral carboranes: the potential for Ïƒ-hole bonding. Physical Chemistry Chemical Physics, 2015, 17, 20814-20821.	1.3	26
78	Insights into Stability and Folding of GNRA and UNCG Tetraloops Revealed by Microsecond Molecular Dynamics and Well-Tempered Metadynamics. Journal of Chemical Theory and Computation, 2015, 11, 3866-3877.	2.3	60
79	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
80	Extensions and applications of the A24 data set of accurate interaction energies. Physical Chemistry Chemical Physics, 2015, 17, 19268-19277.	1.3	50
81	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
82	The Effect of Halogen-to-Hydrogen Bond Substitution on Human Aldose Reductase Inhibition. ACS Chemical Biology, 2015, 10, 1637-1642.	1.6	45
83	Influence of hydrophobic residues on the binding of CB[7] toward diammonium ions of common ammoniumâ‹¯ammonium distance. Organic and Biomolecular Chemistry, 2015, 13, 6249-6254.	1.5	18
84	Large-Scale Quantitative Assessment of Binding Preferences in Proteinâ€"Nucleic Acid Complexes. Journal of Chemical Theory and Computation, 2015, 11, 1939-1948.	2.3	12
85	A comparison of ab initio quantum-mechanical and experimental D₀ binding energies of eleven H-bonded and eleven dispersion-bound complexes. Physical Chemistry Chemical Physics, 2015, 17, 26645-26652.	1.3	16
86	Polar Flattening and the Strength of Halogen Bonding. Journal of Chemical Theory and Computation, 2015, 11, 4727-4732.	2.3	56
87	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
88	Carborane-Based Carbonic Anhydrase Inhibitors: Insight into CAII/CAIX Specificity from a High-Resolution Crystal Structure, Modeling, and Quantum Chemical Calculations. BioMed Research International, 2014, 2014, 1-9.	0.9	18
89	The Dominant Role of Chalcogen Bonding in the Crystal Packing of 2D/3D Aromatics. Angewandte Chemie, 2014, 126, 10303-10306.	1.6	26
90	Characteristics of a Ïƒ-Hole and the Nature of a Halogen Bond. Topics in Current Chemistry, 2014, 359, 1-25.	4.0	19

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91	On the origin of the substantial stabilisation of the electron-donor 1,3-dithiole-2-thione-4-carboxylic acidâ‹†I‹sub›2‹/sub›and DABCOâ‹†I‹sub›2‹/sub›complexes. Physical Chemistry Chemical Physics, 2014, 16, 6679-6686.	1.3	31
92	Statistical analysis of Ïƒ-holes: a novel complementary view on halogen bonding. Physical Chemistry Chemical Physics, 2014, 16, 19111-19114.	1.3	23
93	Selective induced polarization through electron transfer in acetone and pyrazole ester derivatives via Câ€“Hâ‹¯Oî€€ interaction. New Journal of Chemistry, 2014, 38, 4885-4892.	1.4	10
94	The strength and directionality of a halogen bond are co-determined by the magnitude and size of the Ïƒ-hole. Physical Chemistry Chemical Physics, 2014, 16, 9987-9996.	1.3	131
95	Halogen bonds in crystal TTF derivatives: an ab initio quantum mechanical study. Physical Chemistry Chemical Physics, 2014, 16, 2038-2047.	1.3	46
96	Quantum Monte Carlo for noncovalent interactions: an efficient protocol attaining benchmark accuracy. Physical Chemistry Chemical Physics, 2014, 16, 20915-20923.	1.3	46
97	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
98	The nature of bonding and electronic properties of graphene and benzene with iridium adatoms. Physical Chemistry Chemical Physics, 2014, 16, 20818-20827.	1.3	10
99	The Dominant Role of Chalcogen Bonding in the Crystal Packing of 2D/3D Aromatics. Angewandte Chemie - International Edition, 2014, 53, 10139-10142.	7.2	124
100	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
101	Theoretical insight into the stabilization of triazole fungicides via their interactions with dications. International Journal of Mass Spectrometry, 2014, 359, 38-43.	0.7	12
102	Why Is the L-Shaped Structure of X‹sub›2‹/sub›Â·Â·Â·X‹sub›2‹/sub› (X = F, Cl, Br, I) Complexes More Stable Than Other Structures?. Journal of Physical Chemistry A, 2014, 118, 3846-3855.	1.1	21
103	The Dominant Role of Chalcogen Bonding in the Crystal Packing of 2D/3D Aromatics. Angewandte Chemie - International Edition, 2014, 53, 10139-10142.	7.2	1
104	On the Importance and Origin of Aromatic Interactions in Chemistry and Biodisciplines. Accounts of Chemical Research, 2013, 46, 927-936.	7.6	206
105	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
106	Accuracy of Quantum Chemical Methods for Large Noncovalent Complexes. Journal of Chemical Theory and Computation, 2013, 9, 3364-3374.	2.3	275
107	The relative roles of electrostatics and dispersion in the stabilization of halogen bonds. Physical Chemistry Chemical Physics, 2013, 15, 17742.	1.3	129
108	Competition between halogen, dihalogen and hydrogen bonds in bromo- and iodomethanol dimers. Journal of Molecular Modeling, 2013, 19, 2879-2883.	0.8	18

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109	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
110	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
111	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
112	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
113	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
114	Modulation of Aldose Reductase Inhibition by Halogen Bond Tuning. ACS Chemical Biology, 2013, 8, 2484-2492.	1.6	85
115	Quantum Monte Carlo Methods Describe Noncovalent Interactions with Subchemical Accuracy. Journal of Chemical Theory and Computation, 2013, 9, 4287-4292.	2.3	88
116	On the nature of unusual intensity changes in the infrared spectra of the enfluraneâ‹¯acetone complexes. Physical Chemistry Chemical Physics, 2013, 15, 6001.	1.3	14
117	Plugging the explicit Ïƒ-holes in molecular docking. Chemical Communications, 2013, 49, 981-983.	2.2	72
118	Spin-Crossing in an Organometallic Ptâ€“Benzene Complex. Journal of Chemical Theory and Computation, 2013, 9, 1461-1468.	2.3	19
119	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
120	The Semiempirical Quantum Mechanical Scoring Function for In Silico Drug Design. ChemPlusChem, 2013, 78, 921-931.	1.3	80
121	Assessing the Accuracy and Performance of Implicit Solvent Models for Drug Molecules: Conformational Ensemble Approaches. Journal of Physical Chemistry B, 2013, 117, 5950-5962.	1.2	60
122	Quantification of the Interaction Forces between Metals and Graphene by Quantum Chemical Calculations and Dynamic Force Measurements under Ambient Conditions. ACS Nano, 2013, 7, 1646-1651.	7.3	73
123	On the Association of the Base Pairs on the Silica Surface Based on Free Energy Biased Molecular Dynamics Simulation and Quantum Mechanical Calculations. Journal of Physical Chemistry C, 2013, 117, 11066-11075.	1.5	10
124	Differences in the Sublimation Energy of Benzene and Hexahalogenbenzenes Are Caused by Dispersion Energy. Journal of Physical Chemistry A, 2013, 117, 4331-4337.	1.1	20
125	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
126	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

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127	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
128	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
129	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
130	Interaction of Graphene and Arenes with Noble Metals. Journal of Physical Chemistry C, 2012, 116, 14151-14162.	1.5	45
131	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
132	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
133	Benchmark Calculations of Noncovalent Interactions of Halogenated Molecules. Journal of Chemical Theory and Computation, 2012, 8, 4285-4292.	2.3	264
134	Functionalization of Graphene: Covalent and Non-Covalent Approaches, Derivatives and Applications. Chemical Reviews, 2012, 112, 6156-6214.	23.0	3,531
135	Adsorption of Organic Electron Acceptors on Graphene-like Molecules: Quantum Chemical and Molecular Mechanical Study. Journal of Physical Chemistry C, 2012, 116, 25328-25336.	1.5	23
136	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
137	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
138	Calculations on Noncovalent Interactions and Databases of Benchmark Interaction Energies. Accounts of Chemical Research, 2012, 45, 663-672.	7.6	184
139	On Extension of the Current Biomolecular Empirical Force Field for the Description of Halogen Bonds. Journal of Chemical Theory and Computation, 2012, 8, 1325-1333.	2.3	127
140	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
141	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
142	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
143	On the Role of London Dispersion Forces in Biomolecular Structure Determination. Journal of Physical Chemistry B, 2011, 115, 8038-8046.	1.2	41
144	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

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145	Autobiography of Pavel Hobza. Journal of Physical Chemistry A, 2011, 115, 11115-11118.	1.1	0
146	A Ï€-stacked phenylacetylene dimer. Physical Chemistry Chemical Physics, 2011, 13, 16706.	1.3	33
147	The calculation of intermolecular interaction energies. Annual Reports on the Progress of Chemistry Section C, 2011, 107, 148.	4.4	29
148	Halogen bonded complexes between volatile anaesthetics (chloroform, halothane, enflurane,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 622	1.3	44
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