Pavel Hobza

List of Publications by Year in Descending Order

531 papers	46,812 citations	105 h-index	201 g-index
576 ext. papers	49,438 ext. citations	6.5 avg, IF	7.81 L-index

#	Paper	IF	Citations
531	P-Doped graphene-C nanocomposite: a donor-acceptor complex with a P-C dative bond.. *Chemical Communications*, **2022**,	5.8	2
530	The stability of covalent dative bond significantly increases with increasing solvent polarity.. *Nature Communications*, **2022**, 13, 2107	17.4	3
529	Real-space imaging of anisotropic charge of □hole by means of Kelvin probe force microscopy. *Science*, **2021**, 374, 863-867	33.3	18
528	Cyclo[]carbons Form Strong N -> C Dative/Covalent Bonds with Piperidine. *Journal of Physical Chemistry A*, **2021**, 125, 2923-2931	2.8	6
527	The Structure-Based Design of SARS-CoV-2 nsp14 Methyltransferase Ligands Yields Nanomolar Inhibitors. *ACS Infectious Diseases*, **2021**, 7, 2214-2220	5.5	13
526	Addition Reaction between Piperidine and C to Form 1,4-Disubstituted C Proceeds through van der Waals and Dative Bond Complexes: Theoretical and Experimental Study. *Journal of the American Chemical Society*, **2021**, 143, 10930-10939	16.4	3
525	The Existence of a N->C Dative Bond in the C60□Piperidine Complex. *Angewandte Chemie*, **2021**, 133, 1970-1978	3.6	3
524	The Existence of a N->C Dative Bond in the C -Piperidine Complex. *Angewandte Chemie - International Edition*, **2021**, 60, 1942-1950	16.4	10
523	Multipodal insulin mimetics built on adamantane or proline scaffolds. *Bioorganic Chemistry*, **2021**, 107, 104548	5.1	0
522	Tuning the P-C dative/covalent bond formation in RP-C complexes by changing the R group. *Chemical Communications*, **2021**, 57, 3363-3366	5.8	2
521	Structure-directed formation of the dative/covalent bonds in complexes with Cpiperidine. *Physical Chemistry Chemical Physics*, **2021**, 23, 4365-4375	3.6	6
520	Benchmark Data Sets of Boron Cluster Dihydrogen Bonding for the Validation of Approximate Computational Methods. *ChemPhysChem*, **2020**, 21, 2599-2604	3.2	2
519	SQM/COSMO Scoring Function: Reliable Quantum-Mechanical Tool for Sampling and Ranking in Structure-Based Drug Design. *ChemPlusChem*, **2020**, 85, 2362-2371	2.8	3
518	Optimization of norbornyl-based carbocyclic nucleoside analogs as cyclin-dependent kinase 2 inhibitors. *Journal of Molecular Recognition*, **2020**, 33, e2842	2.6	1
517	Mechanical force-induced manipulation of electronic conductance in a spin-crossover complex: a simple approach to molecular electronics. *Nanoscale Advances*, **2020**, 2, 2907-2913	5.1	2
516	Spin modification of iron(ii) 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	4.3	4
515	SQM/COSMO Scoring Function: Reliable Quantum-Mechanical Tool for Sampling and Ranking in Structure-Based Drug Design. *ChemPlusChem*, **2020**, 85, 2361	2.8	0

514	Ground state of the Fe(ii)-porphyrin model system corresponds to quintet: a DFT and DMRG-based tailored CC study. *Physical Chemistry Chemical Physics*, **2020**, 22, 17033-17037	3.6	10
513	Directly linked metalloporphyrins: a quest for bio-inspired materials. *Materials Advances*, **2020**, 1, 1895-1908	3.9	1
512	Chelating Polymers for Hereditary Hemochromatosis Treatment. *Macromolecular Bioscience*, **2020**, 20, e2000254	5.5	1
511	Spin Crossover in Iron(II) Porphyrazine Induced by Noncovalent Interactions Combined with Hybridization of Iron(II) Porphyrazine and Ligand Orbitals: CASPT2, CCSD(T), and DFT Studies. *Journal of Physical Chemistry C*, **2019**, 123, 23186-23194	3.8	4
510	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	5.4	10
509	Structure and Properties of Double-Sandwich Complexes at the Graphene Surface: A Theoretical Study. *Journal of Physical Chemistry C*, **2019**, 123, 14712-14724	3.8	3
508	Chalcogen Bonding due to the Exo-Substitution of Icosahedral Dicarbaborane. *Molecules*, **2019**, 24,	4.8	4
507	Impressive Enrichment of Semiempirical Quantum Mechanics-Based Scoring Function: HSP90 Protein with 4541 Inhibitors and Decoys. *ChemPhysChem*, **2019**, 20, 2721	3.2	1
506	Impressive Enrichment of Semiempirical Quantum Mechanics-Based Scoring Function: HSP90 Protein with 4541 Inhibitors and Decoys. *ChemPhysChem*, **2019**, 20, 2759-2766	3.2	9
505	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	3.8	6
504	Nature of Binding in Planar Halogen Benzene Assemblies and Their Possible Visualization in Scanning Probe Microscopy. *Journal of Physical Chemistry C*, **2019**, 123, 8379-8386	3.8	3
503	Imidazo[1,2-c]pyrimidin-5(6H)-one as a novel core of cyclin-dependent kinase 2 inhibitors: Synthesis, activity measurement, docking, and quantum mechanical scoring. *Journal of Molecular Recognition*, **2018**, 31, e2720	2.6	8
502	Ranking Power of the SQM/COSMO Scoring Function on Carbonic Anhydrase II-Inhibitor Complexes. *ChemPhysChem*, **2018**, 19, 873-879	3.2	22
501	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	3.6	1
500	Sequential BN-doping induced tuning of electronic properties in zigzag-edged graphene nanoribbons: a computational approach.. *RSC Advances*, **2018**, 8, 10964-10974	3.7	1
499	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	3.6	1
498	Interface Interactions of the Bowman 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	3.2	4
497	Quantum Mechanical and Molecular Mechanical Calculations on Substituted Boron Clusters and Their Interactions with Proteins **2018**, 126-138		

496	Non-covalent control of spin-state in metal-organic complex by positioning on N-doped graphene. *Nature Communications*, **2018**, 9, 2831	17.4	52
495	An Isolated Molecule of Iron(II) Phthalocyanin Exhibits Quintet Ground-State: A Nexus between Theory and Experiment. *Chemistry - A European Journal*, **2018**, 24, 13413-13417	4.8	7
494	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	6.4	57
493	S?N chalcogen bonded complexes of carbon disulfide with diazines. Theoretical study. *Chemical Physics*, **2018**, 500, 37-44	2.3	12
492	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	6.4	34
491	SQM/COSMO Scoring Function at the DFTB3-D3H4 Level: Unique Identification of Native Protein-Ligand Poses. *Journal of Chemical Information and Modeling*, **2017**, 57, 127-132	6.1	31
490	Structural Basis of the Interaction of Cyclin-Dependent Kinase 2 with Roscovitine and Its Analogues Having Bioisosteric Central Heterocycles. *ChemPhysChem*, **2017**, 18, 785-795	3.2	11
489	Unraveling the Structure-Affinity Relationship between Cucurbit[n]urils (n = 7, 8) and Cationic Diamondoids. *Journal of the American Chemical Society*, **2017**, 139, 3249-3258	16.4	47
488	Binary twinned-icosahedral [BH] interacts with cyclodextrins as a precedent for its complexation with other organic motifs. *Physical Chemistry Chemical Physics*, **2017**, 19, 11748-11752	3.6	22
487	B-H□a nonclassical hydrogen bond or dispersion contact?. *Physical Chemistry Chemical Physics*, **2017**, 19, 18194-18200	3.6	27
486	Noncovalent Interactions in Specific Recognition Motifs of Protein-DNA Complexes. *Journal of Chemical Theory and Computation*, **2017**, 13, 877-885	6.4	15
485	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	6.8	24
484	Pnictogen bonding in pyrazine□PnX (Pn = P, As, Sb and X = F, Cl, Br) complexes. *Journal of Molecular Modeling*, **2017**, 23, 328	2	16
483	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	3.7	8
482	Selective binding of choline by a phosphate-coordination-based triple helicate featuring an aromatic box. *Nature Communications*, **2017**, 8, 938	17.4	39
481	The Interplay between Various □and □Hole Interactions of Trigonal Boron and Trigonal Pyramidal Arsenic Triiodides. *Crystals*, **2017**, 7, 225	2.3	6
480	Superior Performance of the SQM/COSMO Scoring Functions in Native Pose Recognition of Diverse Protein-Ligand Complexes in Cognate Docking. *ACS Omega*, **2017**, 2, 4022-4029	3.9	17
479	Non-covalent interactions in anisole-(CO) (n = 1, 2) complexes. *Physical Chemistry Chemical Physics*, **2017**, 19, 22749-22758	3.6	2

478	The role of the σ-holes in stability of non-bonded chalcogenidebenzene interactions: the ground and excited states. *Physical Chemistry Chemical Physics*, **2017**, 20, 299-306	3.6	8
477	The SQM/COSMO filter: reliable native pose identification based on the quantum-mechanical description of protein-ligand interactions and implicit COSMO solvation. *Chemical Communications*, **2016**, 52, 3312-5	5.8	46
476	Computational methods for the description of pharmacologically relevant platinum complexes--molecular structure and bond dissociation. *Physical Chemistry Chemical Physics*, **2016**, 18, 4051-62	3.6	3
475	Computer Modeling of Halogen Bonds and Other σ-Hole Interactions. *Chemical Reviews*, **2016**, 116, 5155-87	68.1	444
474	On the nature of the stabilisation of the E[illegible]pnicogen bond in the SbCl3[illegible]toluene complex. *Chemical Communications*, **2016**, 52, 3500-3	5.8	33
473	Benchmark Calculations of Interaction Energies in Noncovalent Complexes and Their Applications. *Chemical Reviews*, **2016**, 116, 5038-71	68.1	267
472	New Insight into the Nature of Bonding in the Dimers of Lappert's Stannylene and Its Ge Analogs: A Quantum Mechanical Study. *Journal of Chemical Theory and Computation*, **2016**, 12, 1696-704	6.4	10
471	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, 462-5	4.3	10
470	IDD388 Polyhalogenated Derivatives as Probes for an Improved Structure-Based Selectivity of AKR1B10 Inhibitors. *ACS Chemical Biology*, **2016**, 11, 2693-2705	4.9	15
469	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	3.5	7
468	Introduction: Noncovalent Interactions. *Chemical Reviews*, **2016**, 116, 4911-2	68.1	83
467	Competition between Halogen, Hydrogen and Dihydrogen Bonding in Brominated Carboranes. *ChemPhysChem*, **2016**, 17, 3373-3376	3.2	37
466	A Nexus between Theory and Experiment: Non-Empirical Quantum Mechanical Computational Methodology Applied to Cucurbit[n]uril?Guest Binding Interactions. *Chemistry - A European Journal*, **2016**, 22, 17226-17238	4.8	19
465	Ab initio and DFT studies of the interaction between carbonyl and thiocarbonyl groups: the role of S[illegible]O chalcogen bonds. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	12
464	Binding energies of the π-stacked anisole dimer: new molecular beam-laser spectroscopy experiments and CCSD(T) calculations. *Chemistry - A European Journal*, **2015**, 21, 6740-6	4.8	18
463	Representative Amino Acid Side-Chain Interactions in Protein-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, 4086-92	6.4	16
462	The properties of substituted 3D-aromatic neutral carboranes: the potential for σ-hole bonding. *Physical Chemistry Chemical Physics*, **2015**, 17, 20814-21	3.6	20
461	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, 3866-77	6.4	39

460	Benchmark Calculations of Three-Body Intermolecular Interactions and the Performance of Low-Cost Electronic Structure Methods. *Journal of Chemical Theory and Computation*, **2015**, 11, 3065-79	6.4	69
459	Extensions and applications of the A24 data set of accurate interaction energies. *Physical Chemistry Chemical Physics*, **2015**, 17, 19268-77	3.6	44
458	Structure and energetics of the anisole-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, 12530-7	3.6	8
457	The Effect of Halogen-to-Hydrogen Bond Substitution on Human Aldose Reductase Inhibition. *ACS Chemical Biology*, **2015**, 10, 1637-42	4.9	45
456	Influence of hydrophobic residues on the binding of CB[7] toward diammonium ions of common ammonium□ammonium distance. *Organic and Biomolecular Chemistry*, **2015**, 13, 6249-54	3.9	11
455	Large-Scale Quantitative Assessment of Binding Preferences in Protein-Nucleic Acid Complexes. *Journal of Chemical Theory and Computation*, **2015**, 11, 1939-48	6.4	8
454	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, 26645-52	3.6	15
453	Polar flattening and the strength of halogen bonding. *Journal of Chemical Theory and Computation*, **2015**, 11, 4727-32	6.4	51
452	Malonate-based inhibitors of mammalian serine racemase: kinetic characterization and structure-based computational study. *European Journal of Medicinal Chemistry*, **2015**, 89, 189-97	6.8	41
451	Binding Energies of the □Stacked Anisole Dimer: New Molecular Beam□Laser Spectroscopy Experiments and CCSD(T) Calculations. *Chemistry - A European Journal*, **2015**, 21, 6637-6637	4.8	3
450	From Dibismuthenes to Three- and Two-Coordinated Bismuthinidenes by Fine Ligand Tuning: Evidence for Aromatic BiC3N Rings through a Combined Experimental and Theoretical Study. *Chemistry - A European Journal*, **2015**, 21, 16917-28	4.8	58
449	Noncovalent Interactions of Heteroboranes. *Challenges and Advances in Computational Chemistry and Physics*, **2015**, 219-239	0.7	4
448	Chalcogen and pnicogen bonds in complexes of neutral icosahedral and bicapped square-antiprismatic heteroboranes. *Journal of Physical Chemistry A*, **2015**, 119, 1388-95	2.8	34
447	Characteristics of a □Hole and the Nature of a Halogen Bond. *Topics in Current Chemistry*, **2015**, 359, 1-25		17
446	On the origin of the substantial stabilisation of the electron-donor 1,3-dithiole-2-thione-4-carboxylic acid□2 and DABCO□2 complexes. *Physical Chemistry Chemical Physics*, **2014**, 16, 6679-86	3.6	26
445	Statistical analysis of □holes: a novel complementary view on halogen bonding. *Physical Chemistry Chemical Physics*, **2014**, 16, 19111-4	3.6	21
444	Selective induced polarization through electron transfer in acetone and pyrazole ester derivatives via C□H?OC interaction. *New Journal of Chemistry*, **2014**, 38, 4885-4892	3.6	10
443	The strength and directionality of a halogen bond are co-determined by the magnitude and size of the □hole. *Physical Chemistry Chemical Physics*, **2014**, 16, 9987-96	3.6	109

442	Halogen bonds in crystal TTF derivatives: an ab initio quantum mechanical study. *Physical Chemistry Chemical Physics*, **2014**, 16, 2038-47	3.6	43
441	Quantum Monte Carlo for noncovalent interactions: an efficient protocol attaining benchmark accuracy. *Physical Chemistry Chemical Physics*, **2014**, 16, 20915-23	3.6	42
440	Evaluation of composite schemes for CCSDT(Q) calculations of interaction energies of noncovalent complexes. *Physical Chemistry Chemical Physics*, **2014**, 16, 19115-21	3.6	15
439	The nature of bonding and electronic properties of graphene and benzene with iridium adatoms. *Physical Chemistry Chemical Physics*, **2014**, 16, 20818-27	3.6	8
438	The dominant role of chalcogen bonding in the crystal packing of 2D/3D aromatics. *Angewandte Chemie - International Edition*, **2014**, 53, 10139-42	16.4	103
437	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, 3066-73	6.4	35
436	Theoretical insight into the stabilization of triazole fungicides via their interactions with dications. *International Journal of Mass Spectrometry*, **2014**, 359, 38-43	1.9	10
435	Why Is the L-Shaped Structure of X⋯X (X = F, Cl, Br, I) Complexes More Stable Than Other Structures?. *Journal of Physical Chemistry A*, **2014**, 118, 3846-3855	2.8	20
434	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, 389869	3	15
433	The Dominant Role of Chalcogen Bonding in the Crystal Packing of 2D/3D Aromatics. *Angewandte Chemie*, **2014**, 126, 10303-10306	3.6	24
432	The Dominant Role of Chalcogen Bonding in the Crystal Packing of 2D/3D Aromatics. *Angewandte Chemie - International Edition*, **2014**, 53, 10139-10142	16.4	1
431	On the importance and origin of aromatic interactions in chemistry and biodisciplines. *Accounts of Chemical Research*, **2013**, 46, 927-36	24.3	171
430	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, 3420-8	6.4	32
429	The accuracy of quantum chemical methods for large noncovalent complexes. *Journal of Chemical Theory and Computation*, **2013**, 9, 3364-3374	6.4	223
428	The relative roles of electrostatics and dispersion in the stabilization of halogen bonds. *Physical Chemistry Chemical Physics*, **2013**, 15, 17742-51	3.6	113
427	Competition between halogen, dihalogen and hydrogen bonds in bromo- and iodomethanol dimers. *Journal of Molecular Modeling*, **2013**, 19, 2879-83	2	18
426	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	1.4	4
425	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, 5296-304	6.4	7

424	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, 14973-82	3.4	40
423	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, 16096-104	3.4	39
422	CCSD[T] Describes Noncovalent Interactions Better than the CCSD(T), CCSD(TQ), and CCSDT Methods. *Journal of Chemical Theory and Computation*, **2013**, 9, 364-9	6.4	57
421	Modulation of aldose reductase inhibition by halogen bond tuning. *ACS Chemical Biology*, **2013**, 8, 2484-92	4.9	75
420	Quantum Monte Carlo Methods Describe Noncovalent Interactions with Subchemical Accuracy. *Journal of Chemical Theory and Computation*, **2013**, 9, 4287-92	6.4	80
419	On the nature of unusual intensity changes in the infrared spectra of the enflurane–acetone complexes. *Physical Chemistry Chemical Physics*, **2013**, 15, 6001-7	3.6	13
418	Plugging the explicit holes in molecular docking. *Chemical Communications*, **2013**, 49, 981-3	5.8	61
417	Spin-Crossing in an Organometallic Pt-Benzene Complex. *Journal of Chemical Theory and Computation*, **2013**, 9, 1461-8	6.4	18
416	Basis Set Dependence of Interaction Energies Computed Using Composite Post-MP2 Methods. *Journal of Chemical Theory and Computation*, **2013**, 9, 330-7	6.4	11
415	The Semiempirical Quantum Mechanical Scoring Function for In Silico Drug Design. *ChemPlusChem*, **2013**, 78, 921-931	2.8	70
414	Assessing the accuracy and performance of implicit solvent models for drug molecules: conformational ensemble approaches. *Journal of Physical Chemistry B*, **2013**, 117, 5950-62	3.4	56
413	Quantification of the interaction forces between metals and graphene by quantum chemical calculations and dynamic force measurements under ambient conditions. *ACS Nano*, **2013**, 7, 1646-51	16.7	60
412	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	3.8	8
411	Differences in the sublimation energy of benzene and hexahalogenbenzenes are caused by dispersion energy. *Journal of Physical Chemistry A*, **2013**, 117, 4331-7	2.8	17
410	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	3.2	61
409	Describing Noncovalent Interactions beyond the Common Approximations: How Accurate Is the "Gold Standard," CCSD(T) at the Complete Basis Set Limit?. *Journal of Chemical Theory and Computation*, **2013**, 9, 2151-5	6.4	305
408	On the performance of the semiempirical quantum mechanical PM6 and PM7 methods for noncovalent interactions. *Chemical Physics Letters*, **2013**, 568-569, 161-166	2.5	85
407	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, 118-29	1.4	50

406	Evaluation of the performance of post-Hartree-Fock methods in terms of intermolecular distance in noncovalent complexes. *Journal of Computational Chemistry*, **2012**, 33, 691-4	3.5	15
405	Advanced Corrections of Hydrogen Bonding and Dispersion for Semiempirical Quantum Mechanical Methods. *Journal of Chemical Theory and Computation*, **2012**, 8, 141-51	6.4	336
404	Interaction of Graphene and Arenes with Noble Metals. *Journal of Physical Chemistry C*, **2012**, 116, 14151-14162	4.8	38
403	Assessment of the performance of MP2 and MP2 variants for the treatment of noncovalent interactions. *Journal of Physical Chemistry A*, **2012**, 116, 4159-69	2.8	101
402	The performance of MP2.5 and MP2.X methods for nonequilibrium geometries of molecular complexes. *Physical Chemistry Chemical Physics*, **2012**, 14, 13187-93	3.6	17
401	Benchmark Calculations of Noncovalent Interactions of Halogenated Molecules. *Journal of Chemical Theory and Computation*, **2012**, 8, 4285-92	6.4	223
400	Functionalization of graphene: covalent and non-covalent approaches, derivatives and applications. *Chemical Reviews*, **2012**, 112, 6156-214	68.1	3041
399	Adsorption of Organic Electron Acceptors on Graphene-like Molecules: Quantum Chemical and Molecular Mechanical Study. *Journal of Physical Chemistry C*, **2012**, 116, 25328-25336	3.8	20
398	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	2.1	9
397	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, 2282-92	6.4	47
396	Calculations on noncovalent interactions and databases of benchmark interaction energies. *Accounts of Chemical Research*, **2012**, 45, 663-72	24.3	160
395	On Extension of the Current Biomolecular Empirical Force Field for the Description of Halogen Bonds. *Journal of Chemical Theory and Computation*, **2012**, 8, 1325-33	6.4	115
394	A stacked phenylacetylene dimer. *Physical Chemistry Chemical Physics*, **2011**, 13, 16706-12	3.6	31
393	The calculation of intermolecular interaction energies. *Annual Reports on the Progress of Chemistry Section C*, **2011**, 107, 148		24
392	Halogen bonded complexes between volatile anaesthetics (chloroform, halothane, enflurane, isoflurane) and formaldehyde: a theoretical study. *Physical Chemistry Chemical Physics*, **2011**, 13, 5105-13	3.6	42
391	Nonadiabatic dynamics of uracil: population split among different decay mechanisms. *Journal of Physical Chemistry A*, **2011**, 115, 5247-55	2.8	77
390	The Nature of the Binding of Au, Ag, and Pd to Benzene, Coronene, and Graphene: From Benchmark CCSD(T) Calculations to Plane-Wave DFT Calculations. *Journal of Chemical Theory and Computation*, **2011**, 7, 3743-3755	6.4	90
389	S66: A Well-balanced Database of Benchmark Interaction Energies Relevant to Biomolecular Structures. *Journal of Chemical Theory and Computation*, **2011**, 7, 2427-2438	6.4	686

388	Free-Energy Simulations of Hydrogen Bonding versus Stacking of Nucleobases on a Graphene Surface. *Journal of Physical Chemistry C*, **2011**, 115, 19455-19462	3.8	23
387	Complete Basis Set Extrapolation and Hybrid Schemes for Geometry Gradients of Noncovalent Complexes. *Journal of Chemical Theory and Computation*, **2011**, 7, 3924-34	6.4	20
386	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	6.4	169
385	Strength and Character of Halogen Bonds in Protein□ligand Complexes. *Crystal Growth and Design*, **2011**, 11, 4272-4278	3.5	76
384	Definition of the hydrogen bond (IUPAC Recommendations 2011). *Pure and Applied Chemistry*, **2011** , 83, 1637-1641	2.1	1111
383	Defining the hydrogen bond: An account (IUPAC Technical Report). *Pure and Applied Chemistry*, **2011**, 83, 1619-1636	2.1	738
382	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		7
381	On the nature of stabilization in weak, medium, and strong charge-transfer complexes: CCSD(T)/CBS and SAPT calculations. *Journal of Physical Chemistry A*, **2011**, 115, 9422-8	2.8	42
380	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, 8581-9	3.4	75
379	Noncovalent interactions in biochemistry. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 3-17	7.9	184
378	Ligand conformational and solvation/desolvation free energy in protein-ligand complex formation. *Journal of Physical Chemistry B*, **2011**, 115, 4718-24	3.4	22
377	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, 223-35	4.2	46
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