Jir Sponer

List of Publications by Citations

396 papers	24,203 citations	76 h-index	141 g-index
432 ext. papers	26,609 ext. citations	6.7 avg, IF	7.01 L-index

#	Paper	IF	Citations
396	Refinement of the AMBER force field for nucleic acids: improving the description of alpha/gamma conformers. *Biophysical Journal*, **2007**, 92, 3817-29	2.9	1705
395	Benchmark database of accurate (MP2 and CCSD(T) complete basis set limit) interaction energies of small model complexes, DNA base pairs, and amino acid pairs. *Physical Chemistry Chemical Physics*, **2006**, 8, 1985-93	3.6	1499
394	Structure, energetics, and dynamics of the nucleic Acid base pairs: nonempirical ab initio calculations. *Chemical Reviews*, **1999**, 99, 3247-76	68.1	932
393	Refinement of the Cornell et al. Nucleic Acids Force Field Based on Reference Quantum Chemical Calculations of Glycosidic Torsion Profiles. *Journal of Chemical Theory and Computation*, **2011**, 7, 2886-2902	6.4	569
392	Density functional theory and molecular clusters. *Journal of Computational Chemistry*, **1995**, 16, 1315-1325	3.5	473
391	Accurate interaction energies of hydrogen-bonded nucleic acid base pairs. *Journal of the American Chemical Society*, **2004**, 126, 10142-51	16.4	413
390	Structures and Energies of Hydrogen-Bonded DNA Base Pairs. A Nonempirical Study with Inclusion of Electron Correlation. *The Journal of Physical Chemistry*, **1996**, 100, 1965-1974		378
389	Nature of Nucleic Acid–Base Stacking: Nonempirical ab Initio and Empirical Potential Characterization of 10 Stacked Base Dimers. Comparison of Stacked and H-Bonded Base Pairs. *The Journal of Physical Chemistry*, **1996**, 100, 5590-5596		376
388	Electronic properties, hydrogen bonding, stacking, and cation binding of DNA and RNA bases. *Biopolymers*, **2001**, 61, 3-31	2.2	374
387	Toward true DNA base-stacking energies: MP2, CCSD(T), and complete basis set calculations. *Journal of the American Chemical Society*, **2002**, 124, 11802-8	16.4	348
386	Nature and magnitude of aromatic stacking of nucleic acid bases. *Physical Chemistry Chemical Physics*, **2008**, 10, 2595-610	3.6	300
385	A systematic molecular dynamics study of nearest-neighbor effects on base pair and base pair step conformations and fluctuations in B-DNA. *Nucleic Acids Research*, **2010**, 38, 299-313	20.1	299
384	Intercalators. 1. Nature of stacking interactions between intercalators (ethidium, daunomycin, ellipticine, and 4',6-diaminide-2-phenylindole) and DNA base pairs. Ab initio quantum chemical, density functional theory, and empirical potential study. *Journal of the American Chemical Society*, **2002**, 124, 9366-76	16.4	275
383	Performance of Molecular Mechanics Force Fields for RNA Simulations: Stability of UUCG and GNRA Hairpins.. *Journal of Chemical Theory and Computation*, **2010**, 6, 3836-3849	6.4	261
382	Refinement of the Sugar-Phosphate Backbone Torsion Beta for AMBER Force Fields Improves the Description of Z- and B-DNA. *Journal of Chemical Theory and Computation*, **2015**, 11, 5723-36	6.4	243
381	Performance of empirical potentials (AMBER, CFF95, CVFF, CHARMM, OPLS, POLTEV), semiempirical quantum chemical methods (AM1, MNDO/M, PM3), and ab initio Hartree–Fock method for interaction of DNA bases: Comparison with nonempirical beyond Hartree–Fock results **1997**, 18, 1136-1150		239
380	RNA Structural Dynamics As Captured by Molecular Simulations: A Comprehensive Overview. *Chemical Reviews*, **2018**, 118, 4177-4338	68.1	235

379	Nonplanar geometries of DNA bases. Ab initio second-order Moeller-Plesset study. *The Journal of Physical Chemistry*, **1994**, 98, 3161-3164		227
378	DNA basepair step deformability inferred from molecular dynamics simulations. *Biophysical Journal*, **2003**, 85, 2872-83	2.9	212
377	Interaction of DNA Base Pairs with Various Metal Cations (Mg2+, Ca2+, Sr2+, Ba2+, Cu+, Ag+, Au+, Zn2+, Cd2+, and Hg2+): Nonempirical ab Initio Calculations on Structures, Energies, and Nonadditivity of the Interaction. *Journal of Physical Chemistry B*, **1997**, 101, 9670-9677	3.4	208
376	Toward Improved Description of DNA Backbone: Revisiting Epsilon and Zeta Torsion Force Field Parameters. *Journal of Chemical Theory and Computation*, **2013**, 9, 2339-2354	6.4	205
375	Nature of base stacking: reference quantum-chemical stacking energies in ten unique B-DNA base-pair steps. *Chemistry - A European Journal*, **2006**, 12, 2854-65	4.8	204
374	Assessing the Current State of Amber Force Field Modifications for DNA. *Journal of Chemical Theory and Computation*, **2016**, 12, 4114-27	6.4	203
373	Hydrogen bonding and stacking of DNA bases: a review of quantum-chemical ab initio studies. *Journal of Biomolecular Structure and Dynamics*, **1996**, 14, 117-35	3.6	202
372	Ab Initio Study of the Interaction of Guanine and Adenine with Various Mono- and Bivalent Metal Cations (Li+, Na+, K+, Rb+, Cs+; Cu+, Ag+, Au+; Mg2+, Ca2+, Sr2+, Ba2+; Zn2+, Cd2+, and Hg2+). *The Journal of Physical Chemistry*, **1996**, 100, 7250-7255		196
371	Reference simulations of noncanonical nucleic acids with different variants of the AMBER force field: quadruplex DNA, quadruplex RNA and Z-DNA. *Journal of Chemical Theory and Computation*, **2012**, 8, 2506-2520	6.4	184
370	DNA base amino groups and their role in molecular interactions: Ab initio and preliminary density functional theory calculations **1996**, 57, 959-970		179
369	H-Bonded and Stacked DNA Base Pairs: Cytosine Dimer. An Ab Initio Second-Order Moeller-Plesset Study. *Journal of the American Chemical Society*, **1995**, 117, 792-798	16.4	177
368	Correlated ab initio study of nucleic acid bases and their tautomers in the gas phase, in a microhydrated environment and in aqueous solution. *Physical Chemistry Chemical Physics*, **2002**, 4, 4192-4203	3.6	175
367	Interaction between the Guanine–Cytosine Watson–Crick DNA Base Pair and Hydrated Group IIa (Mg2+, Ca2+, Sr2+, Ba2+) and Group IIb (Zn2+, Cd2+, Hg2+) Metal Cations. *Journal of Physical Chemistry A*, **1998**, 102, 5951-5957	2.8	166
366	Nanosecond Molecular Dynamics Simulations of Parallel and Antiparallel Guanine Quadruplex DNA Molecules. *Journal of the American Chemical Society*, **1999**, 121, 5519-5534	16.4	153
365	Molecular dynamics and quantum mechanics of RNA: conformational and chemical change we can believe in. *Accounts of Chemical Research*, **2010**, 43, 40-7	24.3	140
364	ABC: a systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. *Nucleic Acids Research*, **2014**, 42, 12272-83	20.1	138
363	Metal-Stabilized Rare Tautomers and Mispairs of DNA Bases: N6-Metalated Adenine and N4-Metalated Cytosine, Theoretical and Experimental Views. *Journal of Physical Chemistry A*, **1999**, 103, 11406-11413	2.8	137
362	Thermodynamic Parameters for Stacking and Hydrogen Bonding of Nucleic Acid Bases in Aqueous Solution: Ab Initio/Langevin Dipoles Study. *Journal of Physical Chemistry B*, **1999**, 103, 884-892	3.4	137

361	Molecular dynamics simulations and thermodynamics analysis of DNA-drug complexes. Minor groove binding between 4',6-diamidino-2-phenylindole and DNA duplexes in solution. *Journal of the American Chemical Society*, **2003**, 125, 1759-69	16.4	136
360	High-energy chemistry of formamide: a unified mechanism of nucleobase formation. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 657-62	11.5	132
359	Sequence-dependent elastic properties of DNA. *Journal of Molecular Biology*, **2000**, 299, 695-709	6.5	132
358	The Effect of Metal Binding to the N7 Site of Purine Nucleotides on Their Structure, Energy, and Involvement in Base Pairing. *Journal of Physical Chemistry B*, **2000**, 104, 7535-7544	3.4	131
357	Molecular dynamics simulations of RNA: an in silico single molecule approach. *Biopolymers*, **2007**, 85, 169-84	2.2	128
356	Bifurcated hydrogen bonds in DNA crystal structures. An ab initio quantum chemical study. *Journal of the American Chemical Society*, **1994**, 116, 709-714	16.4	128
355	Classification and energetics of the base-phosphate interactions in RNA. *Nucleic Acids Research*, **2009**, 37, 4898-918	20.1	126
354	CH···O Contacts in the Adenine···Uracil Watson–Crick and Uracil···Uracil Nucleic Acid Base Pairs: Nonempirical ab Initio Study with Inclusion of Electron Correlation Effects. *Journal of Physical Chemistry B*, **2000**, 104, 6286-6292	3.4	118
353	Cations and hydration in catalytic RNA: molecular dynamics of the hepatitis delta virus ribozyme. *Biophysical Journal*, **2006**, 91, 626-38	2.9	116
352	Formation pathways of a guanine-quadruplex DNA revealed by molecular dynamics and thermodynamic analysis of the substates. *Biophysical Journal*, **2003**, 85, 1787-804	2.9	114
351	Molecular Dynamics Simulations of Nucleic Acids. From Tetranucleotides to the Ribosome. *Journal of Physical Chemistry Letters*, **2014**, 5, 1771-82	6.4	113
350	Single Stranded Loops of Quadruplex DNA As Key Benchmark for Testing Nucleic Acids Force Fields. *Journal of Chemical Theory and Computation*, **2009**, 5, 2514-30	6.4	112
349	Molecular dynamics simulations of Guanine quadruplex loops: advances and force field limitations. *Biophysical Journal*, **2004**, 87, 227-42	2.9	112
348	Base stacking and hydrogen bonding in protonated cytosine dimer: the role of molecular ion-dipole and induction interactions. *Journal of Biomolecular Structure and Dynamics*, **1996**, 13, 695-706	3.6	107
347	Base Pair Fraying in Molecular Dynamics Simulations of DNA and RNA. *Journal of Chemical Theory and Computation*, **2014**, 10, 3177-89	6.4	106
346	Explaining the varied glycosidic conformational, G-tract length and sequence preferences for anti-parallel G-quadruplexes. *Nucleic Acids Research*, **2011**, 39, 4499-512	20.1	105
345	On the potential role of the amino nitrogen atom as a hydrogen bond acceptor in macromolecules. *Journal of Molecular Biology*, **1998**, 279, 1123-36	6.5	105
344	Amino groups in nucleic acid bases, aniline, aminopyridines, and aminotriazine are nonplanar: Results of correlated ab initio quantum chemical calculations and anharmonic analysis of the aniline inversion motion. *Journal of Chemical Physics*, **1996**, 105, 11042-11050	3.9	104

343	Molecular dynamics simulations of G-DNA and perspectives on the simulation of nucleic acid structures. *Methods*, **2012**, 57, 25-39	4.6	103
342	Non-Watson-Crick basepairing and hydration in RNA motifs: molecular dynamics of 5S rRNA loop E. *Biophysical Journal*, **2003**, 84, 3564-82	2.9	101
341	Uracil Dimer: Potential Energy and Free Energy Surfaces. Ab Initio beyond Hartree–Fock and Empirical Potential Studies. *Journal of Physical Chemistry A*, **1998**, 102, 6921-6926	2.8	100
340	Interaction of the Adenine–Thymine Watson–Crick and Adenine–Adenine Reverse-Hoogsteen DNA Base Pairs with Hydrated Group IIa (Mg2+, Ca2+, Sr2+, Ba2+) and IIb (Zn2+, Cd2+, Hg2+) Metal Cations:´Absence of the Base Pair Stabilization by Metal-Induced Polarization Effects. *Journal of Physical Chemistry B*, **1999**, 103, 2528-2534	3.4	98
339	Nonplanar DNA base pairs. *Journal of Biomolecular Structure and Dynamics*, **1996**, 13, 827-33	3.6	95
338	Relative stability of different DNA guanine quadruplex stem topologies derived using large-scale quantum-chemical computations. *Journal of the American Chemical Society*, **2013**, 135, 9785-96	16.4	94
337	Molecular dynamics simulations and their application to four-stranded DNA. *Methods*, **2007**, 43, 278-90	4.6	91
336	Interaction Energies of Hydrogen-Bonded Formamide Dimer, Formamidine Dimer, and Selected DNA Base Pairs Obtained with Large Basis Sets of Atomic Orbitals. *Journal of Physical Chemistry A*, **2000**, 104, 4592-4597	2.8	91
335	Structural dynamics of possible late-stage intermediates in folding of quadruplex DNA studied by molecular simulations. *Nucleic Acids Research*, **2013**, 41, 7128-43	20.1	89
334	Interactions of Hydrated Mg2+ Cation with Bases, Base Pairs, and Nucleotides. Electron Topology, Natural Bond Orbital, Electrostatic, and Vibrational Study. *Journal of Physical Chemistry B*, **2001**, 105, 6051-6060	3.4	89
333	Hinge-like motions in RNA kink-turns: the role of the second a-minor motif and nominally unpaired bases. *Biophysical Journal*, **2005**, 88, 3466-85	2.9	88
332	Comparison of intrinsic stacking energies of ten unique dinucleotide steps in A-RNA and B-DNA duplexes. Can we determine correct order of stability by quantum-chemical calculations?. *Journal of Physical Chemistry B*, **2010**, 114, 1191-203	3.4	87
331	Structural dynamics and cation interactions of DNA quadruplex molecules containing mixed guanine/cytosine quartets revealed by large-scale MD simulations. *Journal of the American Chemical Society*, **2001**, 123, 3295-307	16.4	87
330	Potential Energy Surface of the Cytosine Dimer:´MP2 Complete Basis Set Limit Interaction Energies, CCSD(T) Correction Term, and Comparison with the AMBER Force Field. *Journal of Physical Chemistry B*, **2004**, 108, 5466-5471	3.4	86
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327	A prebiotically plausible synthesis of pyrimidine β-ribonucleosides and their phosphate derivatives involving photoanomerization. *Nature Chemistry*, **2017**, 9, 303-309	17.6	81
326	Nature and magnitude of aromatic base stacking in DNA and RNA: Quantum chemistry, molecular mechanics, and experiment. *Biopolymers*, **2013**, 99, 978-88	2.2	80

325	Crystal structure of d(GGCCAATTGG) complexed with DAPI reveals novel binding mode. *Biochemistry*, **1999**, 38, 16443-51	3.2	79
324	Reference MP2/CBS and CCSD(T) quantum-chemical calculations on stacked adenine dimers. Comparison with DFT-D, MP2.5, SCS(MI)-MP2, M06-2X, CBS(SCS-D) and force field descriptions. *Physical Chemistry Chemical Physics*, **2010**, 12, 3522-34	3.6	78
323	Theoretical Study of Binding of Hydrated Zn(II) and Mg(II) Cations to 5Guanosine Monophosphate. Toward Polarizable Molecular Mechanics for DNA and RNA. *Journal of Physical Chemistry B*, **2003**, 107, 8669-8681	3.4	78
322	A G-quadruplex-binding compound showing anti-tumour activity in an in vivo model for pancreatic cancer. *Scientific Reports*, **2015**, 5, 11385	4.9	77
321	Computer Folding of RNA Tetraloops: Identification of Key Force Field Deficiencies. *Journal of Chemical Theory and Computation*, **2016**, 12, 4534-48	6.4	77
320	Molecular Interactions of Nucleic Acid Bases. A Review of Quantum-Chemical Studies. *Collection of Czechoslovak Chemical Communications*, **2003**, 68, 2231-2282		75
319	Quantum chemical benchmark study on 46 RNA backbone families using a dinucleotide unit. *Journal of Chemical Theory and Computation*, **2015**, 11, 4972-91	6.4	74
318	Theoretical studies of RNA catalysis: hybrid QM/MM methods and their comparison with MD and QM. *Methods*, **2009**, 49, 202-16	4.6	74
317	Non-Watson-Crick base pairing in RNA. quantum chemical analysis of the cis Watson-Crick/sugar edge base pair family. *Journal of Physical Chemistry A*, **2005**, 109, 2292-301	2.8	74
316	Outer-Shell and Inner-Shell Coordination of Phosphate Group to Hydrated Metal Ions (Mg2+, Cu2+, Zn2+, Cd2+) in the Presence and Absence of Nucleobase. The Role of Nonelectrostatic Effects. *Journal of Physical Chemistry B*, **2003**, 107, 1913-1923	3.4	74
315	Molecular Dynamics of Hemiprotonated Intercalated Four-Stranded i-DNA: Stable Trajectories on a Nanosecond Scale. *Journal of the American Chemical Society*, **1998**, 120, 6147-6151	16.4	74
314	Complexes of Pentahydrated Zn2+with Guanine, Adenine, and the GuanineCytosine and AdenineThymine Base Pairs. Structures and Energies Characterized by Polarizable Molecular Mechanics and ab Initio Calculations. *Journal of Physical Chemistry B*, **1999**, 103, 11415-11427	3.4	74
313	Significant structural deformation of nucleic acid bases in stacked base pairs: an ab initio study beyond HartreeFock. *Chemical Physics Letters*, **1998**, 288, 7-14	2.5	73
312	Structure, Stiffness and Substates of the Dickerson-Drew Dodecamer. *Journal of Chemical Theory and Computation*, **2013**, 9, 707-721	6.4	72
311	Extensive molecular dynamics simulations showing that canonical G8 and protonated A38H+ forms are most consistent with crystal structures of hairpin ribozyme. *Journal of Physical Chemistry B*, **2010**, 114, 6642-52	3.4	72
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306	The DNA and RNA sugar-phosphate backbone emerges as the key player. An overview of quantum-chemical, structural biology and simulation studies. *Physical Chemistry Chemical Physics*, **2012**, 14, 15257-77	3.6	68
305	Unique tertiary and neighbor interactions determine conservation patterns of Cis Watson-Crick A/G base-pairs. *Journal of Molecular Biology*, **2003**, 330, 967-78	6.5	68
304	Molecular dynamics of the frame-shifting pseudoknot from beet western yellows virus: the role of non-Watson-Crick base-pairing, ordered hydration, cation binding and base mutations on stability and unfolding. *Journal of Molecular Biology*, **2001**, 313, 1073-91	6.5	68
303	Global Minimum of the Adenine□□Thymine Base Pair Corresponds Neither to Watson□Crick Nor to Hoogsteen Structures. Molecular Dynamic/Quenching/AMBER and ab Initio beyond Hartree□Fock Studies. *Journal of the American Chemical Society*, **2000**, 122, 3495-3499	16.4	67
302	Folding of guanine quadruplex molecules-funnel-like mechanism or kinetic partitioning? An overview from MD simulation studies. *Biochimica Et Biophysica Acta - General Subjects*, **2017**, 1861, 1246-1263	4	66
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300	Large-scale compensation of errors in pairwise-additive empirical force fields: comparison of AMBER intermolecular terms with rigorous DFT-SAPT calculations. *Physical Chemistry Chemical Physics*, **2010**, 12, 10476-93	3.6	65
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298	Structural dynamics of precursor and product of the RNA enzyme from the hepatitis delta virus as revealed by molecular dynamics simulations. *Journal of Molecular Biology*, **2005**, 351, 731-48	6.5	63
297	Critical effect of the N2 amino group on structure, dynamics, and elasticity of DNA polypurine tracts. *Biophysical Journal*, **2002**, 82, 2592-609	2.9	63
296	Dependence of A-RNA simulations on the choice of the force field and salt strength. *Physical Chemistry Chemical Physics*, **2009**, 11, 10701-11	3.6	62
295	Reverse Watson□rick Isocytosine□Cytosine and Guanine□Cytosine Base Pairs Stabilized by the Formation of the Minor Tautomers of Bases. An ab Initio Study in the Gas Phase and in a Water Cluster. *Journal of Physical Chemistry A*, **1998**, 102, 10374-10379	2.8	62
294	Ion Binding to Quadruplex DNA Stems. Comparison of MM and QM Descriptions Reveals Sizable Polarization Effects Not Included in Contemporary Simulations. *Journal of Chemical Theory and Computation*, **2014**, 10, 1326-40	6.4	60
293	Conformational dynamics of the human propeller telomeric DNA quadruplex on a microsecond time scale. *Nucleic Acids Research*, **2013**, 41, 2723-35	20.1	60
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289	Molecular dynamics simulations of RNA kissing-loop motifs reveal structural dynamics and formation of cation-binding pockets. *Nucleic Acids Research*, **2003**, 31, 6942-52	20.1	57
288	Improving the Performance of the Amber RNA Force Field by Tuning the Hydrogen-Bonding Interactions. *Journal of Chemical Theory and Computation*, **2019**, 15, 3288-3305	6.4	56
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285	Insight into G-DNA structural polymorphism and folding from sequence and loop connectivity through free energy analysis. *Journal of the American Chemical Society*, **2011**, 133, 14270-9	16.4	53
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270	Theoretical study of the guanine --> 6-thioguanine substitution in duplexes, triplexes, and tetraplexes. *Journal of the American Chemical Society*, **2004**, 126, 14642-50	16.4	48
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263	Trans Hoogsteen/sugar edge base pairing in RNA. Structures, energies, and stabilities from quantum chemical calculations. *Journal of Physical Chemistry B*, **2009**, 113, 1743-55	3.4	44
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261	The Influence of N7Guanine Modifications on the Strength of Watson□rick Base Pairing and Guanine N1Acidity:´ Comparison of Gas-Phase and Condensed-Phase Trends. *Journal of Physical Chemistry B*, **2003**, 107, 5349-5356	3.4	44
260	Nanosecond Molecular Dynamics of Zipper-like DNA Duplex Structures Containing Sheared G□A Mismatch Pairs. *Journal of the American Chemical Society*, **2000**, 122, 7564-7572	16.4	44
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256	Dynamics of the base of ribosomal A-site finger revealed by molecular dynamics simulations and Cryo-EM. *Nucleic Acids Research*, **2010**, 38, 1325-40	20.1	43
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