YIhan Shao

List of Publications by Year in Descending Order

126 papers	8,734 citations	36 h-index	93 g-index
149 ext. papers	9,788 ext. citations	4.8 avg, IF	5.44 L-index

#	Paper	IF	Citations
126	Cavity quantum-electrodynamical time-dependent density functional theory within Gaussian atomic basis. II. Analytic energy gradient.. *Journal of Chemical Physics*, **2022**, 156, 124104	3.9	1
125	Interactions of N-hydroxyamphetamine with an iron porphyrin: A unique intramolecular H-bond probed by DFT calculations.. *Journal of Inorganic Biochemistry*, **2022**, 231, 111779	4.2	
124	Computational investigation of substituent effects on the fluorescence wavelengths of oxyluciferin analogs. *Journal of Photochemistry and Photobiology A: Chemistry*, **2022**, 431, 114018	4.7	
123	Enhanced Reverse Intersystem Crossing Promoted by Triplet Exciton-Photon Coupling. *Journal of the American Chemical Society*, **2021**, 143, 17786-17792	16.4	2
122	Imaging Autotaxin with F-Labeled Positron Emission Tomography Ligands. *Journal of Medicinal Chemistry*, **2021**, 64, 15053-15068	8.3	0
121	Doubly Polarized QM/MM with Machine Learning Chaperone Polarizability. *Journal of Chemical Theory and Computation*, **2021**,	6.4	2
120	Elucidating the Electronic Structure of a Delayed Fluorescence Emitter via Orbital Interactions, Excitation Energy Components, Charge-Transfer Numbers, and Vibrational Reorganization Energies. *Journal of Physical Chemistry Letters*, **2021**, 12, 2712-2720	6.4	13
119	Plasmon-Induced CO2 Conversion on Al@Cu2O: A DFT Study. *Journal of Physical Chemistry C*, **2021**, 125, 6108-6115	3.8	4
118	Development of a highly-specific F-labeled irreversible positron emission tomography tracer for monoacylglycerol lipase mapping. *Acta Pharmaceutica Sinica B*, **2021**, 11, 1686-1695	15.5	3
117	The Role of Conserved Residues in the DEDDh Motif: the Proton-Transfer Mechanism of HIV-1 RNase H. *ACS Catalysis*, **2021**, 11, 7915-7927	13.1	1
116	Synthesis and preliminary evaluation of novel C-labeled GluN2B-selective NMDA receptor negative allosteric modulators. *Acta Pharmacologica Sinica*, **2021**, 42, 491-498	8	5
115	A simplified charge projection scheme for long-range electrostatics in ab initio QM/MM calculations. *Journal of Chemical Physics*, **2021**, 154, 024115	3.9	7
114	Accelerated Computation of Free Energy Profile at Quantum Mechanical/Molecular Mechanics Accuracy via a Semiempirical Reference Potential. 4. Adaptive QM/MM. *Journal of Chemical Theory and Computation*, **2021**, 17, 1318-1325	6.4	5
113	Reaction Path-Force Matching in Collective Variables: Determining Ab Initio QM/MM Free Energy Profiles by Fitting Mean Force. *Journal of Chemical Theory and Computation*, **2021**, 17, 4961-4980	6.4	6
112	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
111	Quantum-electrodynamical time-dependent density functional theory within Gaussian atomic basis. *Journal of Chemical Physics*, **2021**, 155, 064107	3.9	8
110	On the Accuracy of QM/MM Models: A Systematic Study of Intramolecular Proton Transfer Reactions of Amino Acids in Water. *Journal of Physical Chemistry B*, **2021**, 125, 9304-9316	3.4	1

109	Machine-Learning-Assisted Free Energy Simulation of Solution-Phase and Enzyme Reactions. *Journal of Chemical Theory and Computation*, **2021**, 17, 5745-5758	6.4	14
108	Novel Reversible-Binding PET Ligands for Imaging Monoacylglycerol Lipase Based on the Piperazinyl Azetidine Scaffold. *Journal of Medicinal Chemistry*, **2021**, 64, 14283-14298	8.3	3
107	Development of a triazolobenzodiazepine-based PET probe for subtype-selective vasopressin 1A receptor imaging. *Pharmacological Research*, **2021**, 173, 105886	10.2	3
106	Correction: Analysis and visualization of energy densities. I. Insights from real-time time-dependent density functional theory simulations. *Physical Chemistry Chemical Physics*, **2021**, 23, 8936	3.6	0
105	Affordable Path Integral for Thermodynamic Properties via Molecular Dynamics Simulations Using Semiempirical Reference Potential.. *Journal of Physical Chemistry A*, **2021**, 125, 10677-10685	2.8	1
104	Synthesis and preliminary evaluation of 18F-labeled 1-(6,7-dimethyl-4-(methylamino)-1,3-dihydro-2H-pyrrolo[3,4-c]pyridin-2-yl)-2-(trans-2-(6-fluoropyridin-3-yl)cyclopropyl)et for imaging muscarinic acetylcholine receptor subtype 4. *Tetrahedron Letters*, **2020**, 61, 152060	2	0
103	Synthesis and preliminary evaluation of 4-hydroxy-6-(3-[C]methoxyphenethyl)pyridazin-3(2H)-one, a C-labeled d-amino acid oxidase (DAAO) inhibitor for PET imaging. *Bioorganic and Medicinal Chemistry Letters*, **2020**, 30, 127326	2.9	0
102	TD-DFT spin-adiabats with analytic nonadiabatic derivative couplings. *Journal of Chemical Physics*, **2020**, 152, 044112	3.9	7
101	How accurate are approximate quantum chemical methods at modelling solute-solvent interactions in solvated clusters?. *Physical Chemistry Chemical Physics*, **2020**, 22, 3855-3866	3.6	13
100	Synthesis and pharmacokinetic study of a C-labeled cholesterol 24-hydroxylase inhibitor using Pd-loopP[C]CO fixation method. *Bioorganic and Medicinal Chemistry Letters*, **2020**, 30, 127068	2.9	2
99	Charge reduction in ions in the ionic liquid 1-ethy-2,3-dimethylimidazolium bis(trifluoromethanesulfonyl)imide on the Au(111) surface. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	1
98	Constructing Spin-Adiabatic States for the Modeling of Spin-Crossing Reactions. I. A Shared-Orbital Implementation. *International Journal of Quantum Chemistry*, **2020**, 120, e26123	2.1	1
97	Benchmarking the Performance of Time-Dependent Density Functional Theory Methods on Biochromophores. *Journal of Chemical Theory and Computation*, **2020**, 16, 587-600	6.4	32
96	Accelerated Computation of Free Energy Profile at Quantum Mechanical/Molecular Mechanics Accuracy via a Semiempirical Reference Potential. 3. Gaussian Smoothing on Density-of-States. *Journal of Chemical Theory and Computation*, **2020**, 16, 6814-6822	6.4	5
95	Synthesis and preliminary studies of C-labeled tetrahydro-1,7-naphthyridine-2-carboxamides for PET imaging of metabotropic glutamate receptor 2. *Theranostics*, **2020**, 10, 11178-11196	12.1	5
94	Analysis and visualization of energy densities. I. Insights from real-time time-dependent density functional theory simulations. *Physical Chemistry Chemical Physics*, **2020**, 22, 26838-26851	3.6	3
93	Analysis and visualization of energy densities. II. Insights from linear-response time-dependent density functional theory calculations. *Physical Chemistry Chemical Physics*, **2020**, 22, 26852-26864	3.6	4
92	Turn-on chemiluminescence probes and dual-amplification of signal for detection of amyloid beta species in vivo. *Nature Communications*, **2020**, 11, 4052	17.4	14

91	Identification and Development of a New Positron Emission Tomography Ligand 4-(2-Fluoro-4-[C]methoxyphenyl)-5-((1-methyl-1-pyrazol-3-yl)methoxy)picolinamide for Imaging Metabotropic Glutamate Receptor Subtype 2 (mGlu). *Journal of Medicinal Chemistry*, **2020**, 63, 11469-11483	8.3	2
90	Controlling the Cleavage of Carbon-Carbon Bonds To Generate Difluorobenzyl Carbanions for the Construction of Difluoromethylbenzenes. *Journal of Organic Chemistry*, **2019**, 84, 11665-11675	4.2	3
89	Accelerated computation of free energy profile at ab initio quantum mechanical/molecular mechanical accuracy via a semi-empirical reference potential. II. Recalibrating semi-empirical parameters with force matching. *Physical Chemistry Chemical Physics*, **2019**, 21, 20595-20605	3.6	20
88	Design, Synthesis, and Evaluation of F-Labeled Monoacylglycerol Lipase Inhibitors as Novel Positron Emission Tomography Probes. *Journal of Medicinal Chemistry*, **2019**, 62, 8866-8872	8.3	11
87	Synthesis and Preliminary Evaluations of a Triazole-Cored Antagonist as a PET Imaging Probe ([F]N2B-0518) for GluN2B Subunit in the Brain. *ACS Chemical Neuroscience*, **2019**, 10, 2263-2275	5.7	7
86	Are Explicit Solvent Models More Accurate than Implicit Solvent Models? A Case Study on the Menschutkin Reaction. *Journal of Physical Chemistry A*, **2019**, 123, 5580-5589	2.8	17
85	Computational Insights into Endo/Exo Selectivity of the Diels-Alder Reaction in Explicit Solvent at Ab Initio Quantum Mechanical/Molecular Mechanical Level. *Journal of Physical Chemistry B*, **2019**, 123, 5131-5138	3.4	4
84	Design, Synthesis, and Evaluation of Reversible and Irreversible Monoacylglycerol Lipase Positron Emission Tomography (PET) Tracers Using a "Tail Switching" Strategy on a Piperazinyl Azetidine Skeleton. *Journal of Medicinal Chemistry*, **2019**, 62, 3336-3353	8.3	18
83	Computational modeling of curcumin-based fluorescent probe molecules. *Theoretical Chemistry Accounts*, **2019**, 138, 1	1.9	2
82	Synthesis and Preliminary Evaluation of [C]GNE-1023 as a Potent PET Probe for Imaging Leucine-Rich Repeat Kinase 2 (LRRK2) in Parkinson Disease. *ChemMedChem*, **2019**, 14, 1580-1585	3.7	7
81	Synthesis and Preliminary Evaluation of C-Labeled VU0467485/AZ13713945 and Its Analogues for Imaging Muscarinic Acetylcholine Receptor Subtype 4. *ChemMedChem*, **2019**, 14, 303-309	3.7	4
80	Towards enhanced metabolomic data analysis of mass spectrometry image: Multivariate Curve Resolution and Machine Learning. *Analytica Chimica Acta*, **2018**, 1037, 211-219	6.6	15
79	Synthesis, pharmacology and preclinical evaluation of C-labeled 1,3-dihydro-2H-benzo[d]imidazole-2-ones for imaging -dependent transmembrane AMPA receptor regulatory protein. *European Journal of Medicinal Chemistry*, **2018**, 157, 898-908	6.8	11
78	Representation of the QM Subsystem for Long-Range Electrostatic Interaction in Non-Periodic Ab Initio QM/MM Calculations. *Molecules*, **2018**, 23,	4.8	6
77	Do Better Quality Embedding Potentials Accelerate the Convergence of QM/MM Models? The Case of Solvated Acid Clusters. *Molecules*, **2018**, 23,	4.8	7
76	Efficient Computation of Free Energy Surfaces of Diels?Alder Reactions in Explicit Solvent at Ab Initio QM/MM Level. *Molecules*, **2018**, 23,	4.8	8
75	Accelerated Computation of Free Energy Profile at ab Initio Quantum Mechanical/Molecular Mechanics Accuracy via a Semi-Empirical Reference Potential. I. Weighted Thermodynamics Perturbation. *Journal of Chemical Theory and Computation*, **2018**, 14, 5583-5596	6.4	30
74	Unraveling substituent effects on frontier orbitals of conjugated molecules using an absolutely localized molecular orbital based analysis. *Chemical Science*, **2018**, 9, 8598-8607	9.4	29

73	An Estimation of Hybrid Quantum Mechanical Molecular Mechanical Polarization Energies for Small Molecules Using Polarizable Force-Field Approaches. *Journal of Chemical Theory and Computation*, **2017**, 13, 679-695	6.4	14
72	Performance of the AMOEBA Water Model in the Vicinity of QM Solutes: A Diagnosis Using Energy Decomposition Analysis. *Journal of Chemical Theory and Computation*, **2017**, 13, 1963-1979	6.4	22
71	Efficient Strategy for the Calculation of Solvation Free Energies in Water and Chloroform at the Quantum Mechanical/Molecular Mechanical Level. *Journal of Chemical Information and Modeling*, **2017**, 57, 2476-2489	6.1	23
70	Oxalate-curcumin-based probe for micro- and macroimaging of reactive oxygen species in Alzheimer's disease. *Proceedings of the National Academy of Sciences of the United States of America* , **2017**, 114, 12384-12389	11.5	56
69	An efficient protocol for obtaining accurate hydration free energies using quantum chemistry and reweighting from molecular dynamics simulations. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 4988-4997	3.4	14
68	Calculating distribution coefficients based on multi-scale free energy simulations: an evaluation of MM and QM/MM explicit solvent simulations of water-cyclohexane transfer in the SAMPL5 challenge. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 989-1006	4.2	20
67	Extension of the Effective Fragment Potential Method to Macromolecules. *Journal of Physical Chemistry B*, **2016**, 120, 6562-74	3.4	65
66	Calculations of Solvation Free Energy through Energy Reweighting from Molecular Mechanics to Quantum Mechanics. *Journal of Chemical Theory and Computation*, **2016**, 12, 499-511	6.4	70
65	Computation of Hydration Free Energies Using the Multiple Environment Single System Quantum Mechanical/Molecular Mechanical Method. *Journal of Chemical Theory and Computation*, **2016**, 12, 332-44	6.4	36
64	TINKTEP: A fully self-consistent, mutually polarizable QM/MM approach based on the AMOEBA force field. *Journal of Chemical Physics*, **2016**, 145, 124106	3.9	38
63	Blind prediction of distribution in the SAMPL5 challenge with QM based protomer and pK corrections. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 1087-1100	4.2	24
62	Advanced Potential Energy Surfaces for Molecular Simulation. *Journal of Physical Chemistry B*, **2016**, 120, 9811-32	3.4	66
61	Numerical study on the partitioning of the molecular polarizability into fluctuating charge and induced atomic dipole contributions. *Journal of Physical Chemistry A*, **2015**, 119, 5865-82	2.8	36
60	Superposition of Fragment Excitations for Excited States of Large Clusters with Application to Helium Clusters. *Journal of Chemical Theory and Computation*, **2015**, 11, 5791-803	6.4	13
59	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
58	Efficient treatment of induced dipoles. *Journal of Chemical Physics*, **2015**, 143, 074115	3.9	34
57	Boramino acid as a marker for amino acid transporters. *Science Advances*, **2015**, 1, e1500694	14.3	37
56	Multiple environment single system quantum mechanical/molecular mechanical (MESS-QM/MM) calculations. 1. Estimation of polarization energies. *Journal of Physical Chemistry A*, **2015**, 119, 1511-23	2.8	21

55	Complex absorbing potentials within EOM-CC family of methods: theory, implementation, and benchmarks. *Journal of Chemical Physics*, **2014**, 141, 024102	3.9	84
54	Computing the Free Energy along a Reaction Coordinate Using Rigid Body Dynamics. *Journal of Chemical Theory and Computation*, **2014**, 10, 4198-4207	6.4	13
53	Shared memory multiprocessing implementation of resolution-of-the-identity second-order Møller–Plesset perturbation theory with attenuated and unattenuated results for intermolecular interactions between large molecules. *Molecular Physics*, **2014**, 112, 836-843	1.7	10
52	Analysis of localized diabatic states beyond the condon approximation for excitation energy transfer processes. *Journal of Physical Chemistry A*, **2014**, 118, 11891-900	2.8	7
51	Derivative couplings between TDDFT excited states obtained by direct differentiation in the Tamm-Dancoff approximation. *Journal of Chemical Physics*, **2014**, 141, 024114	3.9	31
50	Effective fragment potential method in Q-CHEM: a guide for users and developers. *Journal of Computational Chemistry*, **2013**, 34, 1060-70	3.5	44
49	Analytic Derivatives of Quartic-Scaling Doubly Hybrid XYGJ-OS Functional: Theory, Implementation, and Benchmark Comparison with M06-2X and MP2 Geometries for Nonbonded Compelexes. *Journal of Chemical Theory and Computation*, **2013**, 9, 1971-1976	6.4	12
48	Accelerating MP2C dispersion corrections for dimers and molecular crystals. *Journal of Chemical Physics*, **2013**, 138, 224112	3.9	30
47	On the structure of Si(100) surface: importance of higher order correlations for buckled dimer. *Journal of Chemical Physics*, **2013**, 138, 204709	3.9	5
46	General implementation of the resolution-of-the-identity and Cholesky representations of electron repulsion integrals within coupled-cluster and equation-of-motion methods: theory and benchmarks. *Journal of Chemical Physics*, **2013**, 139, 134105	3.9	94
45	Comparison of Three Chain-of-States Methods: Nudged Elastic Band and Replica Path with Restraints or Constraints. *Journal of Chemical Theory and Computation*, **2012**, 8, 5035-5051	6.4	20
44	A Quantum Chemical Study of the Ground and Excited State Electronic Structures of Carbazole Oligomers with and without Triarylborane Substitutes. *Journal of Physical Chemistry C*, **2012**, 116, 12434-12442	3.8	17
43	General formulation of spin-flip time-dependent density functional theory using non-collinear kernels: theory, implementation, and benchmarks. *Journal of Chemical Physics*, **2012**, 136, 204103	3.9	163
42	Improved self-consistent and resolution-of-identity approximated Becke–05 density functional model of nondynamic electron correlation. *Journal of Chemical Physics*, **2012**, 136, 034102	3.9	30
41	Communication: Adjusting charge transfer state energies for configuration interaction singles: without any parameterization and with minimal cost. *Journal of Chemical Physics*, **2012**, 136, 161101	3.9	22
40	Ewald mesh method for quantum mechanical calculations. *Journal of Chemical Physics*, **2012**, 136, 114113	3.9	9
39	Efficient Calculation of QM/MM Frequencies with the Mobile Block Hessian. *Journal of Chemical Theory and Computation*, **2011**, 7, 496-514	6.4	29
38	Analytic derivative couplings between configuration-interaction-singles states with built-in electron-translation factors for translational invariance. *Journal of Chemical Physics*, **2011**, 135, 234105	3.9	64

37	Accelerating Correlated Quantum Chemistry Calculations Using Graphical Processing Units and a Mixed Precision Matrix Multiplication Library. *Journal of Chemical Theory and Computation*, **2010**, 6, 135-44	6.4	71
36	A parallel implementation of the analytic nuclear gradient for time-dependent density functional theory within the TammDancoff approximation. *Molecular Physics*, **2010**, 108, 2791-2800	1.7	49
35	Efficient self-consistent DFT calculation of nondynamic correlation based on the B05 method. *Chemical Physics Letters*, **2010**, 493, 381-385	2.5	33
34	Accelerating resolution-of-the-identity second-order MÖller-Plesset quantum chemistry calculations with graphical processing units. *Journal of Physical Chemistry A*, **2008**, 112, 2049-57	2.8	121
33	Vibrational subsystem analysis: A method for probing free energies and correlations in the harmonic limit. *Journal of Chemical Physics*, **2008**, 129, 214109	3.9	47
32	Combined QM/MM calculations of active-site vibrations in binding process of P450cam to putidaredoxin. *Journal of Inorganic Biochemistry*, **2008**, 102, 427-32	4.2	7
31	YinYang atom: a simple combined ab initio quantum mechanical molecular mechanical model. *Journal of Physical Chemistry A*, **2007**, 111, 3661-71	2.8	16
30	Quartic-Scaling Analytical Energy Gradient of Scaled Opposite-Spin Second-Order MÖller-Plesset Perturbation Theory. *Journal of Chemical Theory and Computation*, **2007**, 3, 988-1003	6.4	42
29	Fast evaluation of scaled opposite spin second-order MÖller-Plesset correlation energies using auxiliary basis expansions and exploiting sparsity. *Journal of Computational Chemistry*, **2007**, 28, 1953-64	3.5	53
28	An improved algorithm for analytical gradient evaluation in resolution-of-the-identity second-order MÖller-Plesset perturbation theory: application to alanine tetrapeptide conformational analysis. *Journal of Computational Chemistry*, **2007**, 28, 839-56	3.5	120
27	Dual-basis second-order Moller-Plesset perturbation theory: A reduced-cost reference for correlation calculations. *Journal of Chemical Physics*, **2006**, 125, 074108	3.9	88
26	Dual-basis analytic gradients. 1. Self-consistent field theory. *Journal of Physical Chemistry A*, **2006**, 110, 13915-22	2.8	35
25	A combined density functional theory and molecular mechanics (QM/MM) study of FeCO vibrations in carbonmonoxy myoglobin. *Chemical Physics Letters*, **2006**, 419, 563-566	2.5	15
24	Advances in methods and algorithms in a modern quantum chemistry program package. *Physical Chemistry Chemical Physics*, **2006**, 8, 3172-91	3.6	2371
23	Accurate local approximations to the triples correlation energy: formulation, implementation and tests of 5th-order scaling models. *Molecular Physics*, **2005**, 103, 425-437	1.7	50
22	Lennard-Jones parameters for the combined QM/MM method using the B3LYP/6-31G*/AMBER potential. *Journal of Computational Chemistry*, **2005**, 26, 1270-8	3.5	73
21	Calculating electron transfer couplings by the Spin-Flip approach: energy splitting and dynamical correlation effects. *Chemical Physics Letters*, **2004**, 390, 116-123	2.5	38
20	An efficient method for calculating maxima of homogeneous functions of orthogonal matrices: applications to localized occupied orbitals. *Journal of Chemical Physics*, **2004**, 121, 9220-9	3.9	53

19	Bonding Patterns in Benzene Triradicals from Structural, Spectroscopic, and Thermochemical Perspectives. *Journal of Physical Chemistry A*, **2004**, 108, 6581-6588	2.8	65
18	Fast methods for resumming matrix polynomials and Chebyshev matrix polynomials. *Journal of Computational Physics*, **2004**, 194, 575-587	4.1	13
17	Sparse matrix multiplications for linear scaling electronic structure calculations in an atom-centered basis set using multiatom blocks. *Journal of Computational Chemistry*, **2003**, 24, 618-22	3.5	49
16	Curvy steps for density matrix based energy minimization: tensor formulation and toy applications. *Molecular Physics*, **2003**, 101, 37-43	1.7	22
15	The spin-flip approach within time-dependent density functional theory: Theory and applications to diradicals. *Journal of Chemical Physics*, **2003**, 118, 4807-4818	3.9	489
14	Are both symmetric and buckled dimers on Si(100) minima? Density functional and multireference perturbation theory calculations. *Journal of Chemical Physics*, **2003**, 119, 10917-10923	3.9	42
13	Improved Fermi operator expansion methods for fast electronic structure calculations. *Journal of Chemical Physics*, **2003**, 119, 4117-4125	3.9	76
12	Curvy steps for density matrix-based energy minimization: Application to large-scale self-consistent-field calculations. *Journal of Chemical Physics*, **2003**, 118, 6144-6151	3.9	53
11	Fast evaluation of a linear number of local exchange matrices. *Chemical Physics Letters*, **2002**, 358, 43-50	2.5	17
10	Efficient evaluation of the Coulomb force in density-functional theory calculations. *Journal of Chemical Physics*, **2001**, 114, 6572-6577	3.9	105
9	Q-Chem 2.0: a high-performance ab initio electronic structure program package. *Journal of Computational Chemistry*, **2000**, 21, 1532-1548	3.5	588
8	An improved J matrix engine for density functional theory calculations. *Chemical Physics Letters*, **2000**, 323, 425-433	2.5	46
7	Q-Chem 2.0: a high-performance ab initio electronic structure program package **2000**, 21, 1532		2
6	Enumeration of B24-mNm Cages. *The Journal of Physical Chemistry*, **1996**, 100, 1554-1558		5
5	Enumeration and Symmetry of Substitution Isomers. *The Journal of Physical Chemistry*, **1996**, 100, 15064-15067		5
4	Isomer counting and isomer permutation representation. *Chemical Physics Letters*, **1996**, 248, 366-372	2.5	5
3	The evaluation of moments for benzenoid hydrocarbons. *Theoretica Chimica Acta*, **1995**, 90, 135-144		11
2	Symmetry of hydrogenated C60. *Chemical Physics Letters*, **1995**, 242, 191-195	2.5	15

1 Topology and Stability of Trivalent Polyhedral Clusters. *Fullerenes, Nanotubes, and Carbon Nanostructures*, **1994**, 2, 481-497 6