Julia E Rice

List of Publications by Year in Descending Order

104 papers	8,108 citations	48 h-index	89 g-index
104 ext. papers	8,658 ext. citations	5.5 avg, IF	5.56 L-index

#	Paper	IF	Citations
104	Quantum computation of dominant products in lithium-sulfur batteries. *Journal of Chemical Physics*, **2021**, 154, 134115	3.9	9
103	Computational Investigations of the Lithium Superoxide Dimer Rearrangement on Noisy Quantum Devices. *Journal of Physical Chemistry A*, **2021**, 125, 1827-1836	2.8	11
102	Formation of bis-benzimidazole and bis-benzoxazole through organocatalytic depolymerization of poly(ethylene terephthalate) and its mechanism. *Polymer Chemistry*, **2020**, 11, 4904-4913	4.9	6
101	Quantum orbital-optimized unitary coupled cluster methods in the strongly correlated regime: Can quantum algorithms outperform their classical equivalents?. *Journal of Chemical Physics*, **2020**, 152, 124107	3.9	40
100	Quantum simulation of electronic structure with a transcorrelated Hamiltonian: improved accuracy with a smaller footprint on the quantum computer. *Physical Chemistry Chemical Physics*, **2020**, 22, 24270-24281	3.6	11
99	Reducing Qubit Requirements for Quantum Simulations Using Molecular Point Group Symmetries. *Journal of Chemical Theory and Computation*, **2020**, 16, 6091-6097	6.4	22
98	Influence of Solvent on the Drug-Loading Process of Amphiphilic Nanogel Star Polymers. *Journal of Physical Chemistry B*, **2018**, 122, 5356-5367	3.4	4
97	Identifying Molecular Structural Aromaticity for Hydrocarbon Classification. *ACS Omega*, **2018**, 3, 16035-16039	3.9	8
96	Effect of Hydrophobic Core Topology and Composition on the Structure and Kinetics of Star Polymers: A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2017**, 121, 2902-2918	3.4	5
95	Building a More Predictive Protein Force Field: A Systematic and Reproducible Route to AMBER-FB15. *Journal of Physical Chemistry B*, **2017**, 121, 4023-4039	3.4	147
94	Structural transition of nanogel star polymers with pH by controlling PEGMA interactions with acid or base copolymers. *Molecular Physics*, **2016**, 114, 3221-3231	1.7	8
93	Synthesis of diblock copolymers by combination of organocatalyzed ring-opening polymerization and atom transfer radical polymerization using trichloroethanol as a bifunctional initiator. *Journal of Polymer Science Part A*, **2016**, 54, 563-569	2.5	8
92	Simulation and Experiments To Identify Factors Allowing Synthetic Control of Structural Features of Polymeric Nanoparticles. *Journal of Physical Chemistry B*, **2016**, 120, 7546-68	3.4	3
91	Dominant Decomposition Pathways for Ethereal Solvents in Li-O2 Batteries. *Journal of Physical Chemistry Letters*, **2015**, 6, 1795-9	6.4	40
90	N-Heterocyclic Carbene-Catalyzed Ring Opening Polymerization of ε-Caprolactone with and without Alcohol Initiators: Insights from Theory and Experiment. *Journal of Physical Chemistry B*, **2015**, 119, 5728-37	3.4	32
89	Water soluble, biodegradable amphiphilic polymeric nanoparticles and the molecular environment of hydrophobic encapsulates: Consistency between simulation and experiment. *Polymer*, **2015**, 79, 255-261	3.9	10
88	Role of hydrophilicity and length of diblock arms for determining star polymer physical properties. *Journal of Physical Chemistry B*, **2015**, 119, 944-57	3.4	9

87	Experimental and computational studies on the mechanism of zwitterionic ring-opening polymerization of Ɛvalerolactone with N-heterocyclic carbenes. *Journal of Physical Chemistry B*, **2014**, 118, 6553-60	3.4	48
86	ff14ipq: A Self-Consistent Force Field for Condensed-Phase Simulations of Proteins. *Journal of Chemical Theory and Computation*, **2014**, 10, 4515-4534	6.4	67
85	Tribute to William C. Swope. *Journal of Physical Chemistry B*, **2014**, 118, 6357-9	3.4	
84	Derivation of fixed partial charges for amino acids accommodating a specific water model and implicit polarization. *Journal of Physical Chemistry B*, **2013**, 117, 2328-38	3.4	79
83	Organic acid-catalyzed polyurethane formation via a dual-activated mechanism: unexpected preference of N-activation over O-activation of isocyanates. *Journal of the American Chemical Society*, **2013**, 135, 16235-41	16.4	64
82	Polymerizing Base Sensitive Cyclic Carbonates Using Acid Catalysis.. *ACS Macro Letters*, **2013**, 2, 306-312	6.6	73
81	Advanced chemical recycling of poly(ethylene terephthalate) through organocatalytic aminolysis. *Polymer Chemistry*, **2013**, 4, 1610-1616	4.9	87
80	Unexpected efficiency of cyclic amidine catalysts in depolymerizing poly(ethylene terephthalate). *Journal of Polymer Science Part A*, **2013**, 51, 1606-1611	2.5	38
79	Computational investigations on base-catalyzed diaryl ether formation. *Journal of Organic Chemistry*, **2013**, 78, 5436-43	4.2	15
78	Molecular Dynamics Simulations of Star Polymeric Molecules with Diblock Arms, a Comparative Study. *Journal of Chemical Theory and Computation*, **2012**, 8, 3733-49	6.4	16
77	Catalyst Chelation Effects in Organocatalyzed Ring-Opening Polymerization of Lactide.. *ACS Macro Letters*, **2012**, 1, 19-22	6.6	59
76	Mechanisms of organocatalytic amidation and trans-esterification of aromatic esters as a model for the depolymerization of poly(ethylene) terephthalate. *Journal of Physical Chemistry A*, **2012**, 116, 12389-98	2.8	55
75	QM/MM-Based Fitting of Atomic Polarizabilities for Use in Condensed-Phase Biomolecular Simulation. *Journal of Chemical Theory and Computation*, **2012**, 8, 3839-53	6.4	18
74	Consensus Computational Ligand-Based Design for the Identification of Novel Modulators of Human Estrogen Receptor Alpha. *Molecular Informatics*, **2012**, 31, 246-58	3.8	3
73	Alchemical prediction of hydration free energies for SAMPL. *Journal of Computer-Aided Molecular Design*, **2012**, 26, 551-62	4.2	60
72	Catalytic insights into acid/base conjugates: highly selective bifunctional catalysts for the ring-opening polymerization of lactide. *Chemical Communications*, **2011**, 47, 3105-7	5.8	87
71	Organocatalytic depolymerization of poly(ethylene terephthalate). *Journal of Polymer Science Part A*, **2011**, 49, 1273-1281	2.5	105
70	Accounting for polarization cost when using fixed charge force fields. I. Method for computing energy. *Journal of Physical Chemistry B*, **2010**, 114, 8621-30	3.4	39

69	Acyclic Guanidines as Organic Catalysts for Living Polymerization of Lactide. *Macromolecules*, **2010**, 43, 1660-1664	5.5	67
68	Accounting for polarization cost when using fixed charge force fields. II. Method and application for computing effect of polarization cost on free energy of hydration. *Journal of Physical Chemistry B*, **2010**, 114, 8631-45	3.4	29
67	Hydrogen-bonding catalysts based on fluorinated alcohol derivatives for living polymerization. *Angewandte Chemie - International Edition*, **2009**, 48, 5170-3	16.4	96
66	The reaction mechanism for the organocatalytic ring-opening polymerization of l-lactide using a guanidine-based catalyst: hydrogen-bonded or covalently bound?. *Journal of the American Chemical Society*, **2008**, 130, 6749-54	16.4	205
65	Finding Similar Objects Using a Taxonomy: A Pragmatic Approach. *Lecture Notes in Computer Science*, **2006**, 1039-1057	0.9	2
64	Fast 3D molecular superposition and similarity search in databases of flexible molecules. *Journal of Computer-Aided Molecular Design*, **2003**, 17, 13-38	4.2	32
63	Data management in molecular and cell biology: vision and recommendations. *OMICS A Journal of Integrative Biology*, **2003**, 7, 93-7	3.8	2
62	FLASHFLOOD: a 3D field-based similarity search and alignment method for flexible molecules. *Journal of Computer-Aided Molecular Design*, **2001**, 15, 587-612	4.2	22
61	DiscoveryLink: A system for integrated access to life sciences data sources. *IBM Systems Journal*, **2001**, 40, 489-511		161
60	An analysis of chlorine and bromine oxygen bonding and its implications for stratospheric chemistry. *Molecular Physics*, **1999**, 96, 633-643	1.7	25
59	Design of optimized photorefractive polymers: A novel class of chromophores. *Journal of Chemical Physics*, **1996**, 105, 10637-10647	3.9	89
58	The varying nature of fluorine-oxygen bonds. *Molecular Physics*, **1996**, 89, 1359-1372	1.7	32
57	On the orbital contribution to analytical derivatives of perturbation theory energies. *Molecular Physics*, **1995**, 85, 561-571	1.7	11
56	The molecular structure of cis-FONO. *Chemical Physics Letters*, **1994**, 228, 583-588	2.5	23
55	Measurements and calculations of the hyperpolarizabilities of atoms and small molecules in the gas phase. *Chemical Reviews*, **1994**, 94, 3-29	68.1	472
54	Calculation of vibrational dynamic hyperpolarizabilities for H2O, CO2, and NH3. *Journal of Chemical Physics*, **1993**, 98, 8024-8030	3.9	102
53	A comparison of calculated and experimental hyperpolarizabilities for acetonitrile in gas and liquid phases. *Journal of Chemical Physics*, **1993**, 98, 5595-5603	3.9	77
52	Ab initio study of the chlorine nitrate protonation reaction: implications for loss of ClONO2 in the stratosphere. *The Journal of Physical Chemistry*, **1993**, 97, 6637-6644		40

51	A study of solvent effects on hyperpolarizabilities: The reaction field model applied to acetonitrile. *Journal of Chemical Physics*, **1993**, 99, 426-435	3.9	111
50	Parallel direct SCF and gradient program for workstation clusters. *Journal of Computational Chemistry*, **1993**, 14, 1142-1148	3.5	89
49	Electron correlation effects in hyperpolarizabilities of p-nitroaniline. *The Journal of Physical Chemistry*, **1993**, 97, 1158-1163		222
48	Ab initio study of the molecular structure and vibrational spectrum of nitric acid and its protonated forms. *The Journal of Physical Chemistry*, **1992**, 96, 650-657		59
47	Ab initio determination of the nonlinear optical properties of HCl. *Journal of Chemical Physics*, **1992**, 97, 1138-1143	3.9	50
46	An extensive ab initio study of the structures, vibrational spectra, quadratic force fields, and relative energetics of three isomers of Cl2O2. *Journal of Chemical Physics*, **1992**, 97, 6593-6605	3.9	88
45	Frequency-dependent hyperpolarizabilities for argon, krypton, and neon: Comparison with experiment. *Journal of Chemical Physics*, **1992**, 96, 7580-7586	3.9	40
44	Problems in the comparison of theoretical and experimental hyperpolarizabilities. *Journal of Chemical Physics*, **1992**, 97, 7590-7599	3.9	574
43	FONO: A difficult case for theory and experiment. *Journal of Chemical Physics*, **1992**, 97, 4223-4232	3.9	28
42	Proton affinity of methyl nitrate: less than proton affinity of nitric acid. *Journal of the American Chemical Society*, **1992**, 114, 8247-8256	16.4	39
41	The calculation of frequency-dependent hyperpolarizabilities including electron correlation effects. *International Journal of Quantum Chemistry*, **1992**, 43, 91-118	2.1	107
40	Connected triple excitations in coupled-cluster calculations of hyperpolarizabilities: neon. *Chemical Physics Letters*, **1992**, 191, 23-28	2.5	34
39	Solvent dependence of the second order hyperpolarizability in p-nitroaniline. *Chemical Physics Letters*, **1992**, 191, 245-250	2.5	280
38	Binding energies and bond distances of Ni(CO)x, x=1□4: An application of coupled-cluster theory. *Journal of Chemical Physics*, **1991**, 95, 5898-5905	3.9	78
37	The determination of accurate dipole polarizabilities □and □for the noble gases. *Journal of Chemical Physics*, **1991**, 94, 4972-4979	3.9	104
36	A theoretical study of Na(H2O)+n (n=1□4). *Journal of Chemical Physics*, **1991**, 95, 5142-5148	3.9	131
35	Ion solvation in polarizable water: molecular dynamics simulations. *Journal of the American Chemical Society*, **1991**, 113, 2481-2486	16.4	337
34	The calculation of frequency-dependent polarizabilities as pseudo-energy derivatives. *Journal of Chemical Physics*, **1991**, 94, 4959-4971	3.9	156

33	The energy separation between the classical and nonclassical isomers of protonated acetylene. An extensive study in one- and n-particle space. *Journal of Chemical Physics*, **1991**, 94, 8008-8014	3.9	44
32	Theoretical characterization of tetrahedral N4. *Journal of Chemical Physics*, **1991**, 94, 1215-1221	3.9	121
31	Frequency dependent hyperpolarizabilities with application to formaldehyde and methyl fluoride. *Journal of Chemical Physics*, **1990**, 93, 8828-8839	3.9	121
30	The effect of water models on the interaction of the sodium□chloride ion pair in water: Molecular dynamics simulations. *Journal of Chemical Physics*, **1990**, 93, 7528-7529	3.9	62
29	The polarizabilities of neon. *Chemical Physics Letters*, **1989**, 163, 359-365	2.5	61
28	The structure of cis-butadiene. *Chemical Physics Letters*, **1989**, 161, 277-284	2.5	36
27	Implementation of analytic derivative methods in quantum chemistry. *Computer Physics Reports*, **1989**, 10, 147-187		26
26	Theoretical investigations of molecules composed only of fluorine, oxygen and nitrogen: determination of the equilibrium structures of FOOF, (NO)2 and FNNF and the transition state structure for FNNF cis-trans isomerization. *Theoretica Chimica Acta*, **1989**, 75, 81-98		288
25	Silicocene, (C5H5)2Si: a highly symmetric sandwich compound?. *Journal of the American Chemical Society*, **1989**, 111, 2011-2017	16.4	22
24	The molecular structures and energetics of [7]paracyclophane and [8]paracyclophane. an investigation of the boundaries of aromaticity. *Chemical Physics Letters*, **1988**, 150, 63-70	2.5	15
23	An efficient closed-shell singles and doubles coupled-cluster method. *Chemical Physics Letters*, **1988**, 150, 406-415	2.5	117
22	How bent can a benzene be? The molecular structure, infrared spectrum and energetics of [6]paracyclophane. *Chemical Physics*, **1988**, 123, 1-25	2.3	20
21	Infrared spectrum of F.hivin..cntdot.H2O. *Journal of the American Chemical Society*, **1988**, 110, 6327-6332	16.4	65
20	Second-order perturbation theory and configuration interaction theory applied to medium-sized molecules: cyclopropane, ethylenimine, ethylene oxide, fluoroethane, and acetaldehyde. *Journal of the American Chemical Society*, **1988**, 110, 1388-1393	16.4	43
19	The analytic gradient for the coupled pair functional method: Formula and application for HCl, H2CO, and the dimer H2CO???HCl. *Journal of Chemical Physics*, **1988**, 88, 7011-7023	3.9	33
18	On the necessity of f basis functions for bending frequencies. *Journal of Chemical Physics*, **1988**, 88, 3187-3195	3.9	169
17	A multiconfiguration self-consistent-field (MCSCF) study of the bent and linear conformations of HCCN. *Journal of Chemical Physics*, **1987**, 86, 7051-7053	3.9	44
16	The infrared spectrum of the acetylene radical cation C2H+2. A theoretical study using SCF, MCSCF, and CI methods. *Journal of Chemical Physics*, **1987**, 86, 3051-3053	3.9	36

15	[5]Paracyclophane. An important example of ring strain and aromaticity in hydrocarbon compounds. *Journal of the American Chemical Society*, **1987**, 109, 2902-2909	16.4	49
14	The closed-shell coupled cluster single and double excitation (CCSD) model for the description of electron correlation. A comparison with configuration interaction (CISD) results. *Journal of Chemical Physics*, **1987**, 86, 2881-2890	3.9	291
13	An MCSCF study of the X2B2, 2A2 and 2 2B2 states of benzyl. *Journal of the Chemical Society, Faraday Transactions 2*, **1987**, 83, 1643		29
12	Metaphosphate and tris(methylene)metaphosphate [P(CH2)3-] anions. Do they have three double bonds to phosphorus?. *Journal of the American Chemical Society*, **1987**, 109, 4189-4192	16.4	31
11	Analytic evaluation of energy gradients for the single and double excitation coupled cluster (CCSD) wave function: Theory and application. *Journal of Chemical Physics*, **1987**, 87, 5361-5373	3.9	358
10	Analytic evaluation of energy gradients for the single and double excitation coupled cluster (CCSD) wave function: A comparison with configuration interaction (CCSD, CISDT, and CISDTQ) results for the harmonic vibrational frequencies, infrared intensities, dipole moment, and inversion barrier of ammonia. *International Journal of Quantum Chemistry*, **1987**, 32, 495-501	2.1	25
9	Comparison of single and double excitation coupled cluster and configuration interaction theories: determination of structure and equilibrium propertie. *Chemical Physics Letters*, **1987**, 139, 134-139	2.5	17
8	Molecular structure and infrared spectrum of protonated nitrous oxide. *Chemical Physics Letters*, **1986**, 130, 333-336	2.5	19
7	The analytic configuration interaction gradient method: Application to the cyclic and open isomers of the S3 molecule. *Journal of Chemical Physics*, **1986**, 85, 963-968	3.9	228
6	The efficient evaluation of configuration interaction analytic energy second derivatives: Application to hydrogen thioperoxide, HSOH. *Journal of Chemical Physics*, **1986**, 85, 3930-3938	3.9	46
5	The elimination of singularities in derivative calculations. *Chemical Physics Letters*, **1985**, 120, 151-158	2.5	209
4	On the efficient evaluation of analytic energy gradients. *Chemical Physics Letters*, **1985**, 122, 585-590	2.5	134
3	The low-lying states of silylene. *Chemical Physics Letters*, **1984**, 107, 365-374	2.5	44
2	An analysis of chlorine and bromine oxygen bonding and its implications for stratospheric chemistry		1
1	Emerging quantum computing algorithms for quantum chemistry. *Wiley Interdisciplinary Reviews: Computational Molecular Science*,	7.9	4