# Julia E Rice

## List of Publications by Citations



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|---|---|---|---|
| 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 | Problems in the comparison of theoretical and experimental hyperpolarizabilities. *Journal of Chemical Physics*, **1992**, 97, 7590-7599 | 3.9 | 574 |
| 103 | Measurements and calculations of the hyperpolarizabilities of atoms and small molecules in the gas phase. *Chemical Reviews*, **1994**, 94, 3-29 | 68.1 | 472 |
| 102 | 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 |
| 101 | Ion solvation in polarizable water: molecular dynamics simulations. *Journal of the American Chemical Society*, **1991**, 113, 2481-2486 | 16.4 | 337 |
| 100 | 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 |
| 99 | 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 |
| 98 | Solvent dependence of the second order hyperpolarizability in p-nitroaniline. *Chemical Physics Letters*, **1992**, 191, 245-250 | 2.5 | 280 |
| 97 | 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 |
| 96 | Electron correlation effects in hyperpolarizabilities of p-nitroaniline. *The Journal of Physical Chemistry*, **1993**, 97, 1158-1163 | | 222 |
| 95 | The elimination of singularities in derivative calculations. *Chemical Physics Letters*, **1985**, 120, 151-158 | 2.5 | 209 |
| 94 | 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 |
| 93 | On the necessity of f basis functions for bending frequencies. *Journal of Chemical Physics*, **1988**, 88, 3187-3195 | 3.9 | 169 |
| 92 | DiscoveryLink: A system for integrated access to life sciences data sources. *IBM Systems Journal*, **2001**, 40, 489-511 | | 161 |
| 91 | The calculation of frequency-dependent polarizabilities as pseudo-energy derivatives. *Journal of Chemical Physics*, **1991**, 94, 4959-4971 | 3.9 | 156 |
| 90 | 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 |
| 89 | On the efficient evaluation of analytic energy gradients. *Chemical Physics Letters*, **1985**, 122, 585-590 | 2.5 | 134 |
| 88 | A theoretical study of Na(H2O)+n (n=1–4). *Journal of Chemical Physics*, **1991**, 95, 5142-5148 | 3.9 | 131 |

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| 87 | Frequency dependent hyperpolarizabilities with application to formaldehyde and methyl fluoride. *Journal of Chemical Physics*, **1990**, 93, 8828-8839 | 3.9 | 121 |
| 86 | Theoretical characterization of tetrahedral N4. *Journal of Chemical Physics*, **1991**, 94, 1215-1221 | 3.9 | 121 |
| 85 | An efficient closed-shell singles and doubles coupled-cluster method. *Chemical Physics Letters*, **1988**, 150, 406-415 | 2.5 | 117 |
| 84 | 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 |
| 83 | The calculation of frequency-dependent hyperpolarizabilities including electron correlation effects. *International Journal of Quantum Chemistry*, **1992**, 43, 91-118 | 2.1 | 107 |
| 82 | Organocatalytic depolymerization of poly(ethylene terephthalate). *Journal of Polymer Science Part A*, **2011**, 49, 1273-1281 | 2.5 | 105 |
| 81 | The determination of accurate dipole polarizabilities □ and □ for the noble gases. *Journal of Chemical Physics*, **1991**, 94, 4972-4979 | 3.9 | 104 |
| 80 | Calculation of vibrational dynamic hyperpolarizabilities for H2O, CO2, and NH3. *Journal of Chemical Physics*, **1993**, 98, 8024-8030 | 3.9 | 102 |
| 79 | Hydrogen-bonding catalysts based on fluorinated alcohol derivatives for living polymerization. *Angewandte Chemie - International Edition*, **2009**, 48, 5170-3 | 16.4 | 96 |
| 78 | Design of optimized photorefractive polymers: A novel class of chromophores. *Journal of Chemical Physics*, **1996**, 105, 10637-10647 | 3.9 | 89 |
| 77 | Parallel direct SCF and gradient program for workstation clusters. *Journal of Computational Chemistry*, **1993**, 14, 1142-1148 | 3.5 | 89 |
| 76 | 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 |
| 75 | Advanced chemical recycling of poly(ethylene terephthalate) through organocatalytic aminolysis. *Polymer Chemistry*, **2013**, 4, 1610-1616 | 4.9 | 87 |
| 74 | 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 |
| 73 | 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 |
| 72 | 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 |
| 71 | 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 |
| 70 | Polymerizing Base Sensitive Cyclic Carbonates Using Acid Catalysis.. *ACS Macro Letters*, **2013**, 2, 306-312 | 6.6 | 73 |

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| 69 | 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 |
| 68 | Acyclic Guanidines as Organic Catalysts for Living Polymerization of Lactide. *Macromolecules*, **2010**, 43, 1660-1664 | 5.5 | 67 |
| 67 | Infrared spectrum of F.hivin..cntdot.H2O. *Journal of the American Chemical Society*, **1988**, 110, 6327-6332 | 16.4 | 65 |
| 66 | 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 |
| 65 | 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 |
| 64 | The polarizabilities of neon. *Chemical Physics Letters*, **1989**, 163, 359-365 | 2.5 | 61 |
| 63 | Alchemical prediction of hydration free energies for SAMPL. *Journal of Computer-Aided Molecular Design*, **2012**, 26, 551-62 | 4.2 | 60 |
| 62 | Catalyst Chelation Effects in Organocatalyzed Ring-Opening Polymerization of Lactide.. *ACS Macro Letters*, **2012**, 1, 19-22 | 6.6 | 59 |
| 61 | 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 |
| 60 | 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 |
| 59 | Ab initio determination of the nonlinear optical properties of HCl. *Journal of Chemical Physics*, **1992**, 97, 1138-1143 | 3.9 | 50 |
| 58 | [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 |
| 57 | Experimental and computational studies on the mechanism of zwitterionic ring-opening polymerization of valerolactone with N-heterocyclic carbenes. *Journal of Physical Chemistry B*, **2014**, 118, 6553-60 | 3.4 | 48 |
| 56 | 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 |
| 55 | 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 |
| 54 | 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 |
| 53 | The low-lying states of silylene. *Chemical Physics Letters*, **1984**, 107, 365-374 | 2.5 | 44 |
| 52 | 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 |

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| 51 | Dominant Decomposition Pathways for Ethereal Solvents in Li-O2 Batteries. *Journal of Physical Chemistry Letters*, **2015**, 6, 1795-9 | 6.4 | 40 |
| 50 | 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 |
| 49 | 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 |
| 48 | Frequency-dependent hyperpolarizabilities for argon, krypton, and neon: Comparison with experiment. *Journal of Chemical Physics*, **1992**, 96, 7580-7586 | 3.9 | 40 |
| 47 | 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 |
| 46 | 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 |
| 45 | Unexpected efficiency of cyclic amidine catalysts in depolymerizing poly(ethylene terephthalate). *Journal of Polymer Science Part A*, **2013**, 51, 1606-1611 | 2.5 | 38 |
| 44 | The structure of cis-butadiene. *Chemical Physics Letters*, **1989**, 161, 277-284 | 2.5 | 36 |
| 43 | 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 |
| 42 | Connected triple excitations in coupled-cluster calculations of hyperpolarizabilities: neon. *Chemical Physics Letters*, **1992**, 191, 23-28 | 2.5 | 34 |
| 41 | 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 |
| 40 | N-Heterocyclic Carbene-Catalyzed Ring Opening Polymerization of □Caprolactone with and without Alcohol Initiators: Insights from Theory and Experiment. *Journal of Physical Chemistry B*, **2015**, 119, 5728-37 | 3.4 | 32 |
| 39 | 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 |
| 38 | The varying nature of fluorine-oxygen bonds. *Molecular Physics*, **1996**, 89, 1359-1372 | 1.7 | 32 |
| 37 | 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 |
| 36 | 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 |
| 35 | 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 |
| 34 | FONO: A difficult case for theory and experiment. *Journal of Chemical Physics*, **1992**, 97, 4223-4232 | 3.9 | 28 |

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| 33 | Implementation of analytic derivative methods in quantum chemistry. *Computer Physics Reports*, **1989**, 10, 147-187 | | 26 |
| 32 | An analysis of chlorine and bromine oxygen bonding and its implications for stratospheric chemistry. *Molecular Physics*, **1999**, 96, 633-643 | 1.7 | 25 |
| 31 | 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 |
| 30 | The molecular structure of cis-FONO. *Chemical Physics Letters*, **1994**, 228, 583-588 | 2.5 | 23 |
| 29 | 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 |
| 28 | Silicocene, (C5H5)2Si: a highly symmetric sandwich compound?. *Journal of the American Chemical Society*, **1989**, 111, 2011-2017 | 16.4 | 22 |
| 27 | Reducing Qubit Requirements for Quantum Simulations Using Molecular Point Group Symmetries. *Journal of Chemical Theory and Computation*, **2020**, 16, 6091-6097 | 6.4 | 22 |
| 26 | 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 |
| 25 | Molecular structure and infrared spectrum of protonated nitrous oxide. *Chemical Physics Letters*, **1986**, 130, 333-336 | 2.5 | 19 |
| 24 | 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 |
| 23 | 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 |
| 22 | 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 |
| 21 | Computational investigations on base-catalyzed diaryl ether formation. *Journal of Organic Chemistry*, **2013**, 78, 5436-43 | 4.2 | 15 |
| 20 | 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 |
| 19 | On the orbital contribution to analytical derivatives of perturbation theory energies. *Molecular Physics*, **1995**, 85, 561-571 | 1.7 | 11 |
| 18 | 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 |
| 17 | Computational Investigations of the Lithium Superoxide Dimer Rearrangement on Noisy Quantum Devices. *Journal of Physical Chemistry A*, **2021**, 125, 1827-1836 | 2.8 | 11 |
| 16 | Water soluble, biodegradable amphiphilic polymeric nanoparticles and the molecular environment of hydrophobic encapsulates: Consistency between simulation and experiment. *Polymer*, **2015**, 79, 255-267 | 3.9 | 10 |

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| 15 | 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 |
| 14 | Quantum computation of dominant products in lithium-sulfur batteries. *Journal of Chemical Physics* , **2021**, 154, 134115 | 3.9 | 9 |
| 13 | 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 |
| 12 | 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 |
| 11 | Identifying Molecular Structural Aromaticity for Hydrocarbon Classification. *ACS Omega*, **2018**, 3, 16035-16039 | 3.9 | 8 |
| 10 | 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 |
| 9 | 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 |
| 8 | 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 |
| 7 | Emerging quantum computing algorithms for quantum chemistry. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, | 7.9 | 4 |
| 6 | 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 |
| 5 | 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 |
| 4 | Data management in molecular and cell biology: vision and recommendations. *OMICS A Journal of Integrative Biology*, **2003**, 7, 93-7 | 3.8 | 2 |
| 3 | Finding Similar Objects Using a Taxonomy: A Pragmatic Approach. *Lecture Notes in Computer Science*, **2006**, 1039-1057 | 0.9 | 2 |
| 2 | An analysis of chlorine and bromine oxygen bonding and its implications for stratospheric chemistry | | 1 |
| 1 | Tribute to William C. Swope. *Journal of Physical Chemistry B*, **2014**, 118, 6357-9 | 3.4 | |