Anna I Krylov

List of Publications by Citations

259 papers	18,506 citations	67 h-index	129 g-index
278 ext. papers	20,446 ext. citations	5.6 avg, IF	7.23 L-index

#	Paper	IF	Citations
259	Advances in methods and algorithms in a modern quantum chemistry program package. *Physical Chemistry Chemical Physics*, **2006**, 8, 3172-91	3.6	2371
258	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
257	Equation-of-motion coupled-cluster methods for open-shell and electronically excited species: the Hitchhiker's guide to Fock space. *Annual Review of Physical Chemistry*, **2008**, 59, 433-62	15.7	709
256	Q-Chem 2.0: a high-performance ab initio electronic structure program package. *Journal of Computational Chemistry*, **2000**, 21, 1532-1548	3.5	588
255	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
254	Size-consistent wave functions for bond-breaking: the equation-of-motion spin-flip model. *Chemical Physics Letters*, **2001**, 338, 375-384	2.5	393
253	Singlet-triplet gaps in diradicals by the spin-flip approach: A benchmark study. *Journal of Chemical Physics*, **2002**, 117, 4694-4708	3.9	294
252	Equation-of-motion spin-flip coupled-cluster model with single and double substitutions: Theory and application to cyclobutadiene. *Journal of Chemical Physics*, **2004**, 120, 175-85	3.9	269
251	Q-Chem: an engine for innovation. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 317-326	7.9	257
250	Spin-flip equation-of-motion coupled-cluster electronic structure method for a description of excited states, bond breaking, diradicals, and triradicals. *Accounts of Chemical Research*, **2006**, 39, 83-91	24.3	249
249	Spin-flip configuration interaction: an electronic structure model that is both variational and size-consistent. *Chemical Physics Letters*, **2001**, 350, 522-530	2.5	236
248	Energies and analytic gradients for a coupled-cluster doubles model using variational Brueckner orbitals: Application to symmetry breaking in O4+. *Journal of Chemical Physics*, **1998**, 109, 4171-4181	3.9	216
247	Size-consistent wave functions for nondynamical correlation energy: The valence active space optimized orbital coupled-cluster doubles model. *Journal of Chemical Physics*, **1998**, 109, 10669-10678	3.9	211
246	Dyson orbitals for ionization from the ground and electronically excited states within equation-of-motion coupled-cluster formalism: theory, implementation, and examples. *Journal of Chemical Physics*, **2007**, 127, 234106	3.9	206
245	Singlet Fission in a Covalently Linked Cofacial Alkynyltetracene Dimer. *Journal of the American Chemical Society*, **2016**, 138, 617-27	16.4	204
244	Perturbative corrections to the equation-of-motion spin-flip self-consistent field model: Application to bond-breaking and equilibrium properties of diradicals. *Journal of Chemical Physics*, **2002**, 116, 3194-3203	3.9	180
243	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

242	Fission of Entangled Spins: An Electronic Structure Perspective. *Journal of Physical Chemistry Letters*, **2013**, 4, 3845-3852	6.4	162
241	Photoinduced Chemistry in Fluorescent Proteins: Curse or Blessing?. *Chemical Reviews*, **2017**, 117, 758-795	53.1	154
240	Second-order perturbation corrections to singles and doubles coupled-cluster methods: General theory and application to the valence optimized doubles model. *Journal of Chemical Physics*, **2000**, 113, 3548-3560	3.9	151
239	Cross sections and photoelectron angular distributions in photodetachment from negative ions using equation-of-motion coupled-cluster Dyson orbitals. *Journal of Chemical Physics*, **2009**, 131, 124114	3.9	150
238	Femtosecond multidimensional imaging of a molecular dissociation. *Science*, **2006**, 311, 219-22	33.3	150
237	A spin-complete version of the spin-flip approach to bond breaking: What is the impact of obtaining spin eigenfunctions?. *Journal of Chemical Physics*, **2003**, 118, 9084-9094	3.9	133
236	Shape of Multireference, Equation-of-Motion Coupled-Cluster, and Density Functional Theory Potential Energy Surfaces at a Conical Intersection. *Journal of Chemical Theory and Computation*, **2014**, 10, 3074-84	6.4	132
235	A noniterative perturbative triples correction for the spin-flipping and spin-conserving equation-of-motion coupled-cluster methods with single and double substitutions. *Journal of Chemical Physics*, **2008**, 129, 194105	3.9	126
234	Excited states theory for optimized orbitals and valence optimized orbitals coupled-cluster doubles models. *Journal of Chemical Physics*, **2000**, 113, 6509-6527	3.9	122
233	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
232	Quantum chemistry behind bioimaging: insights from ab initio studies of fluorescent proteins and their chromophores. *Accounts of Chemical Research*, **2012**, 45, 265-75	24.3	114
231	Calculations predict a stable molecular crystal of N8. *Nature Chemistry*, **2014**, 6, 52-6	17.6	107
230	Quantum Chemical Benchmark Studies of the Electronic Properties of the Green Fluorescent Protein Chromophore. 1. Electronically Excited and Ionized States of the Anionic Chromophore in the Gas Phase. *Journal of Chemical Theory and Computation*, **2009**, 5, 1895-906	6.4	104
229	A Simple Kinetic Model for Singlet Fission: A Role of Electronic and Entropic Contributions to Macroscopic Rates. *Journal of Physical Chemistry C*, **2014**, 118, 5188-5195	3.8	103
228	Spin-conserving and spin-flipping equation-of-motion coupled-cluster method with triple excitations. *Journal of Chemical Physics*, **2005**, 123, 084107	3.9	102
227	On the electronically excited states of uracil. *Journal of Physical Chemistry A*, **2008**, 112, 9983-92	2.8	101
226	Extending Quantum Chemistry of Bound States to Electronic Resonances. *Annual Review of Physical Chemistry*, **2017**, 68, 525-553	15.7	97
225	Photoelectron wave function in photoionization: plane wave or Coulomb wave?. *Journal of Physical Chemistry Letters*, **2015**, 6, 4532-40	6.4	97

224	Benchmarking Excited-State Calculations Using Exciton Properties. *Journal of Chemical Theory and Computation*, **2018**, 14, 710-725	6.4	97
223	Potential Energy Landscape of the Electronic States of the GFP Chromophore in Different Protonation Forms: Electronic Transition Energies and Conical Intersections. *Journal of Chemical Theory and Computation*, **2010**, 6, 2377-87	6.4	95
222	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
221	Noncovalent interactions in extended systems described by the effective fragment potential method: theory and application to nucleobase oligomers. *Journal of Physical Chemistry A*, **2010**, 114, 12739-54	2.8	91
220	Linker-Dependent Singlet Fission in Tetracene Dimers. *Journal of the American Chemical Society*, **2018**, 140, 10179-10190	16.4	90
219	Interacting Rydberg and valence states in radicals and molecules: experimental and theoretical studies. *International Reviews in Physical Chemistry*, **2009**, 28, 267-308	7	89
218	New implementation of high-level correlated methods using a general block tensor library for high-performance electronic structure calculations. *Journal of Computational Chemistry*, **2013**, 34, 2293-2309	3.5	88
217	New and Efficient Equation-of-Motion Coupled-Cluster Framework for Core-Excited and Core-Ionized States. *Journal of Chemical Theory and Computation*, **2019**, 15, 3117-3133	6.4	86
216	Frozen natural orbitals for ionized states within equation-of-motion coupled-cluster formalism. *Journal of Chemical Physics*, **2010**, 132, 014109	3.9	85
215	Complex absorbing potentials within EOM-CC family of methods: theory, implementation, and benchmarks. *Journal of Chemical Physics*, **2014**, 141, 024102	3.9	84
214	First-principle protocol for calculating ionization energies and redox potentials of solvated molecules and ions: theory and application to aqueous phenol and phenolate. *Journal of Physical Chemistry B*, **2012**, 116, 7269-80	3.4	84
213	Effect of solvation on the vertical ionization energy of thymine: from microhydration to bulk. *Journal of Physical Chemistry A*, **2011**, 115, 6028-38	2.8	84
212	The effect of pi-stacking, H-bonding, and electrostatic interactions on the ionization energies of nucleic acid bases: adenine-adenine, thymine-thymine and adenine-thymine dimers. *Physical Chemistry Chemical Physics*, **2010**, 12, 2292-307	3.6	83
211	Electronic structure of the trimethylenemethane diradical in its ground and electronically excited states: Bonding, equilibrium geometries, and vibrational frequencies. *Journal of Chemical Physics*, **2003**, 118, 6874-6883	3.9	83
210	A Fresh Look at Resonances and Complex Absorbing Potentials: Density Matrix-Based Approach. *Journal of Physical Chemistry Letters*, **2014**, 5, 310-5	6.4	82
209	Effect of protein environment on electronically excited and ionized states of the green fluorescent protein chromophore. *Journal of Physical Chemistry B*, **2011**, 115, 8296-303	3.4	82
208	Electronic structure and spectroscopy of nucleic acid bases: ionization energies, ionization-induced structural changes, and photoelectron spectra. *Journal of Physical Chemistry A*, **2010**, 114, 12305-17	2.8	82
207	Double spin-flip approach within equation-of-motion coupled cluster and configuration interaction formalisms: Theory, implementation, and examples. *Journal of Chemical Physics*, **2009**, 130, 044103	3.9	82

206	On couplings and excimers: lessons from studies of singlet fission in covalently linked tetracene dimers. *Physical Chemistry Chemical Physics*, **2016**, 18, 7751-61	3.6	81
205	Benchmark full configuration interaction and equation-of-motion coupled-cluster model with single and double substitutions for ionized systems results for prototypical charge transfer systems: noncovalent ionized dimers. *Journal of Chemical Physics*, **2007**, 127, 164110	3.9	81
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199	Mapping the Excited State Potential Energy Surface of a Retinal Chromophore Model with Multireference and Equation-of-Motion Coupled-Cluster Methods. *Journal of Chemical Theory and Computation*, **2013**, 9, 4495-506	6.4	76
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196	Observation of the fastest chemical processes in the radiolysis of water. *Science*, **2020**, 367, 179-182	33.3	74
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193	Spin-orbit couplings within the equation-of-motion coupled-cluster framework: Theory, implementation, and benchmark calculations. *Journal of Chemical Physics*, **2015**, 143, 064102	3.9	68
192	Extension of the Effective Fragment Potential Method to Macromolecules. *Journal of Physical Chemistry B*, **2016**, 120, 6562-74	3.4	65
191	Bonding Patterns in Benzene Triradicals from Structural, Spectroscopic, and Thermochemical Perspectives. *Journal of Physical Chemistry A*, **2004**, 108, 6581-6588	2.8	65
190	Non-Condon Effects in the One- and Two-Photon Absorption Spectra of the Green Fluorescent Protein. *Journal of Physical Chemistry Letters*, **2011**, 2, 488-492	6.4	63
189	Ionization of dimethyluracil dimers leads to facile proton transfer in the absence of hydrogen bonds. *Nature Chemistry*, **2012**, 4, 323-9	17.6	62

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187	Spin-flip methods in quantum chemistry. *Physical Chemistry Chemical Physics*, **2020**, 22, 4326-4342	3.6	61
186	Spectroscopic signatures of proton transfer dynamics in the water dimer cation. *Journal of Chemical Physics*, **2010**, 132, 194311	3.9	59
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183	Electronic structure of the benzene dimer cation. *Journal of Chemical Physics*, **2007**, 127, 044317	3.9	56
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176	Perspective: Computational chemistry software and its advancement as illustrated through three grand challenge cases for molecular science. *Journal of Chemical Physics*, **2018**, 149, 180901	3.9	49
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174	Multiheme Cytochrome Mediated Redox Conduction through Shewanella oneidensis MR-1 Cells. *Journal of the American Chemical Society*, **2018**, 140, 10085-10089	16.4	48
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172	Perturbative triples correction for the equation-of-motion coupled-cluster wave functions with single and double substitutions for ionized states: Theory, implementation, and examples. *Journal of Chemical Physics*, **2009**, 131, 114112	3.9	47
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158	Quantifying charge resonance and multiexciton character in coupled chromophores by charge and spin cumulant analysis. *Journal of Chemical Physics*, **2015**, 142, 224104	3.9	40
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141	General framework for calculating spin-orbit couplings using spinless one-particle density matrices: Theory and application to the equation-of-motion coupled-cluster wave functions. *Journal of Chemical Physics*, **2019**, 151, 034106	3.9	33
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