UÄur Bozkaya

List of Publications by Year
in descending order

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62 papers	2,702 citations	218677 26 h-index	182427 51 g-index
74 all docs	74 docs citations	74 times ranked	2811 citing authors

#	Article	IF	Citations
1	<scp>Psi4</scp> 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. Journal of Chemical Theory and Computation, 2017, 13, 3185-3197.	5.3	961
2	P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	3.0	440
3	Quadratically convergent algorithm for orbital optimization in the orbital-optimized coupled-cluster doubles method and in orbital-optimized second-order MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2011, 135, 104103.	3.0	104
4	Orbital-Optimized Second-Order Perturbation Theory with Density-Fitting and Cholesky Decomposition Approximations: An Efficient Implementation. Journal of Chemical Theory and Computation, 2014, 10, 2371-2378.	5.3	58
5	Orbital-optimized third-order MÃ¸ller-Plesset perturbation theory and its spin-component and spin-opposite scaled variants: Application to symmetry breaking problems. Journal of Chemical Physics, 2011, 135, 224103.	3.0	52
6	Symmetric and asymmetric triple excitation corrections for the orbital-optimized coupled-cluster doubles method: Improving upon CCSD(T) and CCSD(T)Î›: Preliminary application. Journal of Chemical Physics, 2012, 136, 204114.	3.0	52
7	Orbital-optimized coupled-electron pair theory and its analytic gradients: Accurate equilibrium geometries, harmonic vibrational frequencies, and hydrogen transfer reactions. Journal of Chemical Physics, 2013, 139, 054104.	3.0	48
8	Analytic energy gradients for the orbital-optimized second-order MÃ¸llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 2013, 138, 184103.	3.0	48
9	Novel phenomena for aggregation induced emission enhancement: highly fluorescent hydrophobic TPE-BODIPY couples in both organic and aqueous media. RSC Advances, 2013, 3, 15866.	3.6	44
10	Network structure and swelling behavior of poly(acrylamide/crotonic acid) hydrogels in aqueous salt solutions. Journal of Polymer Science, Part B: Polymer Physics, 2003, 41, 1656-1664.	2.1	43
11	Derivation of general analytic gradient expressions for density-fitted post-Hartree-Fock methods: An efficient implementation for the density-fitted second-order MÃ¸llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 2014, 141, 124108.	3.0	41
12	Orbital-Optimized MP3 and MP2.5 with Density-Fitting and Cholesky Decomposition Approximations. Journal of Chemical Theory and Computation, 2016, 12, 1179-1188.	5.3	40
13	The extended Koopmans' theorem for orbital-optimized methods: Accurate computation of ionization potentials. Journal of Chemical Physics, 2013, 139, 154105.	3.0	38
14	Transition Metal Cationâ^Ï€ Interactions: Complexes Formed by Fe2+, Co2+, Ni2+, Cu2+, and Zn2+ Binding with Benzene Molecules. Journal of Physical Chemistry A, 2017, 121, 6500-6509.	2.5	36
15	The barrier height, unimolecular rate constant, and lifetime for the dissociation of HN2. Journal of Chemical Physics, 2010, 132, 064308.	3.0	35
16	Analytic Energy Gradients and Spin Multiplicities for Orbital-Optimized Second-Order Perturbation Theory with Density-Fitting Approximation: An Efficient Implementation. Journal of Chemical Theory and Computation, 2014, 10, 4389-4399.	5.3	34
17	Analytic energy gradients for the coupled-cluster singles and doubles with perturbative triples method with the density-fitting approximation. Journal of Chemical Physics, 2017, 147, 044104.	3.0	34
18	Assessment of Orbital-Optimized Third-Order MÃ¸llerâ€“Plesset Perturbation Theory and Its Spin-Component and Spin-Opposite Scaled Variants for Thermochemistry and Kinetics. Journal of Chemical Theory and Computation, 2013, 9, 1452-1460.	5.3	33

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19	Orbital-optimized MP2.5 and its analytic gradients: Approaching CCSD(T) quality for noncovalent interactions. Journal of Chemical Physics, 2014, 141, 204105.	3.0	32
20	Analytic energy gradients for the coupled-cluster singles and doubles method with the density-fitting approximation. Journal of Chemical Physics, 2016, 144, 174103.	3.0	32
21	Accurate Electron Affinities from the Extended Koopmansâ€™ Theorem Based on Orbital-Optimized Methods. Journal of Chemical Theory and Computation, 2014, 10, 2041-2048.	5.3	31
22	Orbital-optimized linearized coupled-cluster doubles with density-fitting and Cholesky decomposition approximations: an efficient implementation. Physical Chemistry Chemical Physics, 2016, 18, 11362-11373.	2.8	30
23	Analytic energy gradients for the orbital-optimized third-order MÃ¸llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 2013, 139, 104116.	3.0	29
24	The lowest-lying electronic singlet and triplet potential energy surfaces for the HNOâ€“NOH system: Energetics, unimolecular rate constants, tunneling and kinetic isotope effects for the isomerization and dissociation reactions. Journal of Chemical Physics, 2012, 136, 164303.	3.0	28
25	Accurate Open-Shell Noncovalent Interaction Energies from the Orbital-Optimized MÃ¸llerâ€“Plesset Perturbation Theory: Achieving CCSD Quality at the MP2 Level by Orbital Optimization. Journal of Chemical Theory and Computation, 2013, 9, 4679-4683.	5.3	28
26	Assessment of Orbital-Optimized MP2.5 for Thermochemistry and Kinetics: Dramatic Failures of Standard Perturbation Theory Approaches for Aromatic Bond Dissociation Energies and Barrier Heights of Radical Reactions. Journal of Chemical Theory and Computation, 2015, 11, 1564-1573.	5.3	28
27	Dihydroxylation of olefins catalyzed by zeolite-confined osmium(0) nanoclusters: an efficient and reusable method for the preparation of 1,2-cis-diols. Green Chemistry, 2012, 14, 1488.	9.0	27
28	Assessment of the extended Koopmans' theorem for the chemical reactivity: Accurate computations of chemical potentials, chemical hardnesses, and electrophilicity indices. Journal of Computational Chemistry, 2016, 37, 345-353.	3.3	20
29	Assessment of the orbitalâ€optimized coupledâ€electron pair theory for thermochemistry and kinetics: Improving on CCSD and CEPA(1). Journal of Computational Chemistry, 2014, 35, 1073-1081.	3.3	18
30	Analytic energy gradients for orbitalâ€optimized MP3 and MP2.5 with the densityâ€fitting approximation: An efficient implementation. Journal of Computational Chemistry, 2018, 39, 351-360.	3.3	18
31	Potential Energy Surfaces for Rearrangements of Berson Trimethylenemethanes. Journal of Physical Chemistry A, 2012, 116, 2309-2321.	2.5	15
32	A noniterative asymmetric triple excitation correction for the density-fitted coupled-cluster singles and doubles method: Preliminary applications. Journal of Chemical Physics, 2016, 144, 144108.	3.0	15
33	Efficient and automated computation of accurate molecular geometries using focal-point approximations to large-basis coupled-cluster theory. Journal of Chemical Physics, 2020, 152, 124109.	3.0	15
34	Theoretical Study of Thermal Rearrangements of 1-Hexen-5-yne, 1,2,5-Hexatriene, and 2-Methylenebicyclo[2.1.0]pentane. Journal of Organic Chemistry, 2012, 77, 2337-2344.	3.2	14
35	Dihydropyridazine-appended dibenzosuberenones as a new class of fluorophores: Application to fluoride sensing. Tetrahedron Letters, 2017, 58, 2981-2985.	1.4	14
36	State-of-the-Art Computations of Vertical Ionization Potentials with the Extended Koopmansâ€™ Theorem Integrated with the CCSD(T) Method. Journal of Physical Chemistry A, 2018, 122, 4375-4380.	2.5	13

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37	Efficient Implementation of the Second-Order Quasidegenerate Perturbation Theory with Density-Fitting and Cholesky Decomposition Approximations: Is It Possible To Use Hartreeâ€“Fock Orbitals for a Multiconfigurational Perturbation Theory?. Journal of Chemical Theory and Computation, 2019, 15, 4415-4429.	5.3	13
38	Energy and analytic gradients for the orbital-optimized coupled-cluster doubles method with the density-fitting approximation: An efficient implementation. Journal of Chemical Physics, 2020, 153, 244115.	3.0	12
39	Thermal Rearrangements of 1-Ethynyl-2-methylcyclopropane: A Computational Study. Journal of Physical Chemistry A, 2012, 116, 3274-3281.	2.5	11
40	Aza-Nazarov Cyclization Reactions via Anion Exchange Catalysis. Organic Letters, 2019, 21, 554-558.	4.6	11
41	Thermal Aromatizations of 2-Vinylmethylenecyclopropane and 3-Vinylcyclobutene. Journal of Organic Chemistry, 2012, 77, 5714-5723.	3.2	10
42	Anionic water pentamer and hexamer clusters: An extensive study of structures and energetics. Journal of Chemical Physics, 2018, 148, 124307.	3.0	9
43	Thermal denitrogenation of 7-isopropylidene-2,3-diaza-norbornene: formation of substituted 3-methylene-(1,4)-pentadienes. Physical Chemistry Chemical Physics, 2012, 14, 14282.	2.8	8
44	Stateâ€ofâ€theâ€art computations of dipole moments using analytic gradients of highâ€level densityâ€fitted coupledâ€cluster methods with focalâ€point approximations. Journal of Computational Chemistry, 2020, 41, 769-779.	3.3	5
45	Ionized water clusters , n = 2 to 6: A highâ€accuracy study of structures and energetics. International Journal of Quantum Chemistry, 2020, 120, e26100.	2.0	5
46	Computational Study for the Reaction Mechanism of N-Hydroxyphthalimide-Catalyzed Oxidative Cleavage of Alkenes. Journal of Organic Chemistry, 2020, 85, 10136-10142.	3.2	5
47	Polarizationâ€Enhanced Hydrogen Bonding in 1,8â€Dihydroxynaphthalene: Conformational Analysis, Binding Studies and Hydrogen Bonding Catalysis. ChemistrySelect, 2020, 5, 13387-13396.	1.5	5
48	Assessment of the Density-Fitted Second-Order Quasidegenerate Perturbation Theory for Transition Energies: Accurate Computations of Singletâ€“Triplet Gaps for Charge-Transfer Compounds. Journal of Physical Chemistry A, 2020, 124, 6889-6898.	2.5	5
49	Conformational Characterization of Polyelectrolyte Oligomers and Their Noncovalent Complexes Using Ion Mobility-Mass Spectrometry. Journal of the American Society for Mass Spectrometry, 2020, 31, 441-449.	2.8	5
50	Efficient implementations of the symmetric and asymmetric triple excitation corrections for the orbital-optimized coupled-cluster doubles method with the density-fitting approximation. Journal of Chemical Physics, 2021, 155, 114104.	3.0	5
51	The ten chemically transparent dinitronaphthalene isomers and their radical anions. Molecular Physics, 2010, 108, 2491-2509.	1.7	4
52	Chargeâ€Transfer Complex of pâ€Aminodiphenylamine with Maleic Anhydride: Spectroscopic, Electrochemical, and Physical Properties. ChemPhysChem, 2016, 17, 2056-2065.	2.1	4
53	State-Of-The-Art Computations of Vertical Electron Affinities with the Extended Koopmansâ€™ Theorem Integrated with the CCSD(T) Method. Journal of Chemical Theory and Computation, 2021, 17, 7648-7656.	5.3	4
54	A rare Î³-pyranopyrazole skeleton: design, one-pot synthesis and computational study. Organic and Biomolecular Chemistry, 2016, 14, 7490-7494.	2.8	3

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55	M<scp>acro</scp>QC 1.0: An electronic structure theory software for large-scale applications. Journal of Chemical Physics, 2022, 156, 044801.	3.0	3
56	Efficient Implementation of Equation-of-Motion Coupled-Cluster Singles and Doubles Method with the Density-Fitting Approximation: An Enhanced Algorithm for the Particleâ€“Particle Ladder Term. Journal of Chemical Theory and Computation, 2022, 18, 1489-1500.	5.3	3
57	An anomalous addition of chlorosulfonyl isocyanate to a carbonyl group: the synthesis of ((3aS,7aR,E)-2-ethyl-3-oxo-2,3,3a,4,7,7a-hexahydro-1H-isoindol-1-ylidene)sulfamoyl chloride. Beilstein Journal of Organic Chemistry, 2019, 15, 931-936.	2.2	2
58	Anharmonic force field from coupled-cluster methods and accurate computation of infrared spectra. Advances in Quantum Chemistry, 2021, 83, 139-153.	0.8	2
59	<scp>Molint</scp> 1.0: A framework for the computation of molecular integrals and their derivatives for <scp>densityâ€fitted</scp> methods. International Journal of Quantum Chemistry, 2021, 121, e26623.	2.0	2
60	Efficient and regioselective synthesis of dihydroxy-substituted 2-aminocyclooctane-1-carboxylic acid and its bicyclic derivatives. Beilstein Journal of Organic Chemistry, 2022, 18, 77-85.	2.2	2
61	Regio- and stereo-chemical ring-opening reactions of the 2,3-epoxy alcohol derivative with nucleophiles: Explanation of the structures and C-2 selectivity supported by theoretical computations. Journal of Molecular Structure, 2022, 1264, 133163.	3.6	2
62	A computational study of the reaction mechanism of 2,2-azobis(isobutyronitrile)-initiated oxidative cleavage of geminal alkenes. Organic and Biomolecular Chemistry, 2021, 19, 9483-9490.	2.8	0