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	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
2	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
3	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
4	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
5	Anharmonic force field from coupled-cluster methods and accurate computation of infrared spectra. Advances in Quantum Chemistry, 2021, 83, 139-153.	0.8	2
6	<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
7	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
8	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
9	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
10	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
11	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
12	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
13	Polarizationâ€Enhanced Hydrogen Bonding in 1,8â€Dihydroxynaphthalene: Conformational Analysis, Binding Studies and Hydrogen Bonding Catalysis. ChemistrySelect, 2020, 5, 13387-13396.	1.5	5
14	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
15	P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	3.0	440
16	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
17	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
18	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

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19	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
20	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
21	Aza-Nazarov Cyclization Reactions via Anion Exchange Catalysis. Organic Letters, 2019, 21, 554-558.	4.6	11
22	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
23	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
24	Anionic water pentamer and hexamer clusters: An extensive study of structures and energetics. Journal of Chemical Physics, 2018, 148, 124307.	3.0	9
25	<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
26	Dihydropyridazine-appended dibenzosuberenones as a new class of fluorophores: Application to fluoride sensing. Tetrahedron Letters, 2017, 58, 2981-2985.	1.4	14
27	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
28	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
29	A rare Î³-pyranopyrazole skeleton: design, one-pot synthesis and computational study. Organic and Biomolecular Chemistry, 2016, 14, 7490-7494.	2.8	3
30	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
31	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
32	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
33	Chargeâ€Transfer Complex of pâ€Aminodiphenylamine with Maleic Anhydride: Spectroscopic, Electrochemical, and Physical Properties. ChemPhysChem, 2016, 17, 2056-2065.	2.1	4
34	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
35	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
36	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

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37	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
38	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
39	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
40	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
41	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
42	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
43	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
44	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
45	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
46	Analytic energy gradients for the orbital-optimized second-order MÃ¸llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 2013, 138, 184103.	3.0	48
47	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
48	The extended Koopmans' theorem for orbital-optimized methods: Accurate computation of ionization potentials. Journal of Chemical Physics, 2013, 139, 154105.	3.0	38
49	Analytic energy gradients for the orbital-optimized third-order MÃ¸llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 2013, 139, 104116.	3.0	29
50	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
51	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
52	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
53	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
54	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

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55	Thermal Aromatizations of 2-Vinylmethylenecyclopropane and 3-Vinylcyclobutene. Journal of Organic Chemistry, 2012, 77, 5714-5723.	3.2	10
56	Thermal Rearrangements of 1-Ethynyl-2-methylcyclopropane: A Computational Study. Journal of Physical Chemistry A, 2012, 116, 3274-3281.	2.5	11
57	Potential Energy Surfaces for Rearrangements of Berson Trimethylenemethanes. Journal of Physical Chemistry A, 2012, 116, 2309-2321.	2.5	15
58	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
59	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
60	The ten chemically transparent dinitronaphthalene isomers and their radical anions. Molecular Physics, 2010, 108, 2491-2509.	1.7	4
61	The barrier height, unimolecular rate constant, and lifetime for the dissociation of HN2. Journal of Chemical Physics, 2010, 132, 064308.	3.0	35
62	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