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Akademik Unvanlar / Görevler

Prof.Dr., Hacettepe Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2020 - Devam Ediyor
Doç.Dr., Hacettepe Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2015 - 2020
Doç.Dr., Atatürk Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2014 - 2015
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Atatürk Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2013 - 2013

Yönetilen Tezler

BOZKAYA U., Optimize orbitalli möller-plesset pertürbasyon ve eşleşmiş elektron çiftleri teorilerinin termokimya ve kinetiğe uygulamaları, Yüksek Lisans, E.SOYDAŞ(Öğrenci), 2015

SCI, SSCI ve AHCI İndekslerine Giren Dergilerde Yayınlanan Makaleler

I. **A computational study of the reaction mechanism of 2,2-azobis(isobutyronitrile)-initiated oxidative cleavage of geminal alkenes**
Essiz S., BOZKAYA U.
ORGANIC & BIOMOLECULAR CHEMISTRY, 2021 (SCI İndekslerine Giren Dergi)

II. **Molint 1.0: A framework for the computation of molecular integrals and their derivatives for density-fitted methods**
BOZKAYA U.
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, 2021 (SCI İndekslerine Giren Dergi)

III. **Energy and analytic gradients for the orbital-optimized coupled-cluster doubles method with the density-fitting approximation: An efficient implementation**
BOZKAYA U., ÜNAL A., Alagoz Y.
JOURNAL OF CHEMICAL PHYSICS, cilt.153, sa.24, 2020 (SCI İndekslerine Giren Dergi)

IV. **Polarization-Enhanced Hydrogen Bonding in 1,8-Dihydroxynaphthalene: Conformational Analysis, Binding Studies and Hydrogen Bonding Catalysis**
Mammadova F., Hamarat B., Ahmadli D., ŞAHİN O., BOZKAYA U., TÜRKMEN Y. E.
CHEMISTRYSELECT, cilt.5, sa.42, ss.13387-13396, 2020 (SCI İndekslerine Giren Dergi)

V. **Computational Study for the Reaction Mechanism of N-Hydroxyphthalimide-Catalyzed Oxidative Cleavage of Alkenes**
EŞSİZ S., BOZKAYA U.
JOURNAL OF ORGANIC CHEMISTRY, cilt.85, sa.15, ss.10136-10142, 2020 (SCI İndekslerine Giren Dergi)

VI. **Assessment of the Density-Fitted Second-Order Quasidegenerate Perturbation Theory for Transition Energies: Accurate Computations of Singlet-Triplet Gaps for Charge-Transfer Compounds**
Servan S. A. , ÜNAL A., Hamarat B., BOZKAYA U.
JOURNAL OF PHYSICAL CHEMISTRY A, cilt.124, sa.34, ss.6889-6898, 2020 (SCI İndekslerine Giren Dergi)

VII. **PSI4 1.4: Open-source software for high-throughput quantum chemistry**
Smith D. G. A. , Burns L. A. , Simmonett A. C. , Parrish R. M. , Schieber M. C. , Galvelis R., Kraus P., Kruse H., Di Remigio R., Alenaizan A., et al.
JOURNAL OF CHEMICAL PHYSICS, cilt.152, sa.18, 2020 (SCI İndekslerine Giren Dergi)

VIII. **Ionized water clusters (H2O)(n)(+), n=2 to 6: A high-accuracy study of structures and energetics**
ÜNAL A., BOZKAYA U.
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, cilt.120, sa.7, 2020 (SCI İndekslerine Giren Dergi)

IX. **Efficient and automated computation of accurate molecular geometries using focal-point approximations to large-basis coupled-cluster theory**
Warden C. E. , Smith D. G. A. , Burns L. A. , BOZKAYA U., Sherrill C. D.
JOURNAL OF CHEMICAL PHYSICS, cilt.152, sa.12, 2020 (SCI İndekslerine Giren Dergi)

X. **State-of-the-art computations of dipole moments using analytic gradients of high-level density-fitted coupled-cluster methods with focal-point approximations**
BOZKAYA U., Soydas E., Filiz B.
JOURNAL OF COMPUTATIONAL CHEMISTRY, cilt.41, sa.8, 2020 (SCI İndekslerine Giren Dergi)

XI. **Conformational Characterization of Polyelectrolyte Oligomers and Their Noncovalent Complexes Using Ion Mobility-Mass Spectrometry**
ATAKAY M., Aksakal F., BOZKAYA U., SALİH B., Wesdemiotis C.
JOURNAL OF THE AMERICAN SOCIETY FOR MASS SPECTROMETRY, cilt.31, sa.2, ss.441-449, 2020 (SCI İndekslerine Giren Dergi)

XII. **Efficient Implementation of the Second-Order Quasidegenerate Perturbation Theory with Density-Fitting and Cholesky Decomposition Approximations: Is It Possible To Use Hartree-Fock Orbitals for a Multiconfigurational Perturbation Theory?**
BOZKAYA U.
JOURNAL OF CHEMICAL THEORY AND COMPUTATION, cilt.15, sa.8, ss.4415-4429, 2019 (SCI İndekslerine Giren Dergi)

XIII. **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**
KÖSE A., ÜNAL A., ŞAHİN E., BOZKAYA U., KARA Y.
BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY, cilt.15, ss.931-936, 2019 (SCI İndekslerine Giren Dergi)

XIV. **Aza-Nazarov Cyclization Reactions via Anion Exchange Catalysis**

Donmez S. E. , Soydas E., Aydin G., ŞAHİN O., BOZKAYA U., TÜRKMEN Y. E.
ORGANIC LETTERS, cilt.21, sa.2, ss.554-558, 2019 (SCI İndekslerine Giren Dergi)

XV. **State-of-the-Art Computations of Vertical Ionization Potentials with the Extended Koopmans' Theorem Integrated with the CCSD(T) Method**
BOZKAYA U., ÜNAL A.
JOURNAL OF PHYSICAL CHEMISTRY A, cilt.122, sa.17, ss.4375-4380, 2018 (SCI İndekslerine Giren Dergi)

XVI. **Analytic Energy Gradients for Orbital-Optimized MP3 and MP2.5 with the Density-Fitting Approximation: An Efficient Implementation**
BOZKAYA U.
JOURNAL OF COMPUTATIONAL CHEMISTRY, cilt.39, sa.7, ss.351-360, 2018 (SCI İndekslerine Giren Dergi)

XVII. **Anionic water pentamer and hexamer clusters: An extensive study of structures and energetics**
ÜNAL A., BOZKAYA U.
JOURNAL OF CHEMICAL PHYSICS, cilt.148, sa.12, 2018 (SCI İndekslerine Giren Dergi)

XVIII. **Transition Metal Cation-pi Interactions: Complexes Formed by Fe2+, Co2+, Ni2+, Cu2+, and Zn2+ Binding with Benzene Molecules**
Demircan C. A. , BOZKAYA U.
JOURNAL OF PHYSICAL CHEMISTRY A, cilt.121, sa.34, ss.6500-6509, 2017 (SCI İndekslerine Giren Dergi)

XIX. **PSI4 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability**
Parrish R. M. , Burns L. A. , Smith D. G. A. , Simmonett A. C. , DePrince A. E. , Hohenstein E. G. , BOZKAYA U., Sokolov A. Y. , Di Remigio R., Richard R. M. , et al.
JOURNAL OF CHEMICAL THEORY AND COMPUTATION, cilt.13, sa.7, ss.3185-3197, 2017 (SCI İndekslerine Giren Dergi)

XX. **Dihydropyridazine-appended dibenzosuberenones as a new class of fluorophores: Application to fluoride sensing**
Kocak R., Yildiz D., BOZKAYA U., DAŞTAN A., BOZDEMİR Ö. A.
TETRAHEDRON LETTERS, cilt.58, sa.30, ss.2981-2985, 2017 (SCI İndekslerine Giren Dergi)

XXI. **Analytic energy gradients for the coupled-cluster singles and doubles with perturbative triples method with the density-fitting approximation**
BOZKAYA U., Sherrill C. D.
JOURNAL OF CHEMICAL PHYSICS, cilt.147, sa.4, 2017 (SCI İndekslerine Giren Dergi)

XXII. **Charge-Transfer Complex of p-Aminodiphenylamine with Maleic Anhydride: Spectroscopic, Electrochemical, and Physical Properties**
KARACA E., Can H., BOZKAYA U., Pekmez N. O.
CHEMPHYSCHEM, cilt.17, sa.13, ss.2056-2065, 2016 (SCI İndekslerine Giren Dergi)

XXIII. **Analytic energy gradients for the coupled-cluster singles and doubles method with the density-fitting approximation**
BOZKAYA U., Sherrill C. D.
JOURNAL OF CHEMICAL PHYSICS, cilt.144, sa.17, 2016 (SCI İndekslerine Giren Dergi)

XXIV. **Orbital-optimized linearized coupled-cluster doubles with density-fitting and Cholesky decomposition approximations: an efficient implementation**
BOZKAYA U.
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, cilt.18, sa.16, ss.11362-11373, 2016 (SCI İndekslerine Giren Dergi)

XXV. **A noniterative asymmetric triple excitation correction for the density-fitted coupled-cluster singles and doubles method: Preliminary applications**
BOZKAYA U.
JOURNAL OF CHEMICAL PHYSICS, cilt.144, sa.14, 2016 (SCI İndekslerine Giren Dergi)

XXVI. **Orbital-Optimized MP3 and MP2.5 with Density-Fitting and Cholesky Decomposition Approximations**
BOZKAYA U.
JOURNAL OF CHEMICAL THEORY AND COMPUTATION, cilt.12, sa.3, ss.1179-1188, 2016 (SCI İndekslerine Giren Dergi)

XXVII. **A rare gamma-pyranopyrazole skeleton: design, one-pot synthesis and computational study**
Ucuncu M., Canturk C., Karakus E., Zeybek H., BOZKAYA U., Soydas E., ŞAHİN E., EMRULLAHOĞLU M.
ORGANIC & BIOMOLECULAR CHEMISTRY, cilt.14, sa.31, ss.7490-7494, 2016 (SCI İndekslerine Giren Dergi)

XXVIII. **Assessment of the extended Koopmans' theorem for the chemical reactivity: Accurate computations of chemical potentials, chemical hardnesses, and electrophilicity indices**
Yildiz D., Bozkaya U.
JOURNAL OF COMPUTATIONAL CHEMISTRY, cilt.37, sa.3, ss.345-353, 2016 (SCI İndekslerine Giren Dergi)

XXIX. **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**
Soydas E., Bozkaya U.
JOURNAL OF CHEMICAL THEORY AND COMPUTATION, cilt.11, sa.4, ss.1564-1573, 2015 (SCI İndekslerine Giren Dergi)

XXX. **Orbital-optimized MP2.5 and its analytic gradients: Approaching CCSD(T) quality for noncovalent interactions**
Bozkaya U., Sherrill C. D.
JOURNAL OF CHEMICAL PHYSICS, cilt.141, sa.20, 2014 (SCI İndekslerine Giren Dergi)

XXXI. **Analytic Energy Gradients and Spin Multiplicities for Orbital-Optimized Second-Order Perturbation Theory with Density-Fitting Approximation: An Efficient Implementation**
Bozkaya U.
JOURNAL OF CHEMICAL THEORY AND COMPUTATION, cilt.10, sa.10, ss.4389-4399, 2014 (SCI İndekslerine Giren Dergi)

XXXII. **Derivation of general analytic gradient expressions for density-fitted post-Hartree-Fock methods: An efficient implementation for the density-fitted second-order Moller-Plesset perturbation theory**
Bozkaya U.
JOURNAL OF CHEMICAL PHYSICS, cilt.141, sa.12, 2014 (SCI İndekslerine Giren Dergi)

XXXIII. **Orbital-Optimized Second-Order Perturbation Theory with Density-Fitting and Cholesky Decomposition Approximations: An Efficient Implementation**
Bozkaya U.
JOURNAL OF CHEMICAL THEORY AND COMPUTATION, cilt.10, sa.6, ss.2371-2378, 2014 (SCI İndekslerine Giren Dergi)

XXXIV. **Accurate Electron Affinities from the Extended Koopmans' Theorem Based on Orbital-Optimized Methods**
Bozkaya U.
JOURNAL OF CHEMICAL THEORY AND COMPUTATION, cilt.10, sa.5, ss.2041-2048, 2014 (SCI İndekslerine Giren Dergi)

XXXV. **Assessment of the Orbital-Optimized Coupled-Electron Pair Theory for Thermochemistry and Kinetics: Improving on CCSD and CEPA(**
Soydas E., Bozkaya U.
JOURNAL OF COMPUTATIONAL CHEMISTRY, cilt.35, sa.14, ss.1073-1081, 2014 (SCI İndekslerine Giren Dergi)

XXXVI. **Accurate Open-Shell Noncovalent Interaction Energies from the Orbital-Optimized Moller-Plesset Perturbation Theory: Achieving CCSD Quality at the MP2 Level by Orbital Optimization**
Soydas E., Bozkaya U.
JOURNAL OF CHEMICAL THEORY AND COMPUTATION, cilt.9, sa.11, ss.4679-4683, 2013 (SCI İndekslerine Giren Dergi)

XXXVII. **The extended Koopmans' theorem for orbital-optimized methods: Accurate computation of ionization potentials**
Bozkaya U.
JOURNAL OF CHEMICAL PHYSICS, cilt.139, sa.15, 2013 (SCI İndekslerine Giren Dergi)

XXXVIII. **Analytic energy gradients for the orbital-optimized third-order Moller-Plesset perturbation theory**
Bozkaya U.

JOURNAL OF CHEMICAL PHYSICS, cilt.139, sa.10, 2013 (SCI İndekslerine Giren Dergi)

XXXIX. **Orbital-optimized coupled-electron pair theory and its analytic gradients: Accurate equilibrium geometries, harmonic vibrational frequencies, and hydrogen transfer reactions**
Bozkaya U., Sherrill C. D.
JOURNAL OF CHEMICAL PHYSICS, cilt.139, sa.5, 2013 (SCI İndekslerine Giren Dergi)

XL. **Analytic energy gradients for the orbital-optimized second-order Moller-Plesset perturbation theory**
Bozkaya U., Sherrill C. D.
JOURNAL OF CHEMICAL PHYSICS, cilt.138, sa.18, 2013 (SCI İndekslerine Giren Dergi)

XLI. **Assessment of Orbital-Optimized Third-Order Moller-Plesset Perturbation Theory and Its Spin-Component and Spin-Opposite Scaled Variants for Thermochemistry and Kinetics**
Soydas E., Bozkaya U.
JOURNAL OF CHEMICAL THEORY AND COMPUTATION, cilt.9, sa.3, ss.1452-1460, 2013 (SCI İndekslerine Giren Dergi)

XLII. **Novel phenomena for aggregation induced emission enhancement: highly fluorescent hydrophobic TPE-BODIPY couples in both organic and aqueous media**
Baglan M., Ozturk S., Gur B., Meral K., Bozkaya U., BOZDEMİR Ö. A. , Atilgan S.
RSC ADVANCES, cilt.3, sa.36, ss.15866-15874, 2013 (SCI İndekslerine Giren Dergi)

XLIII. **Thermal Aromatizations of 2-Vinylmethylenecyclopropane and 3-Vinylcyclobutene**
Bozkaya U., ÖZKAN İ.
JOURNAL OF ORGANIC CHEMISTRY, cilt.77, sa.13, ss.5714-5723, 2012 (SCI İndekslerine Giren Dergi)

XLIV. **Symmetric and asymmetric triple excitation corrections for the orbital-optimized coupled-cluster doubles method: Improving upon CCSD(T) and CCSD(T)(Lambda): Preliminary application**
Bozkaya U., Schaefer H. F.
JOURNAL OF CHEMICAL PHYSICS, cilt.136, sa.20, 2012 (SCI İndekslerine Giren Dergi)

XLV. **The lowest-lying electronic singlet and triplet potential energy surfaces for the HNO-NOH system: Energetics, unimolecular rate constants, tunneling and kinetic isotope effects for the isomerization and dissociation reactions**
Bozkaya U., Turney J. M. , Yamaguchi Y., Schaefer H. F.
JOURNAL OF CHEMICAL PHYSICS, cilt.136, sa.16, 2012 (SCI İndekslerine Giren Dergi)

XLVI. **Theoretical Study of Thermal Rearrangements of 1-Hexen-5-yne, 1,2,5-Hexatriene, and 2-Methylenebicyclo[2.1.0]pentane**
Bozkaya U., ÖZKAN İ.
JOURNAL OF ORGANIC CHEMISTRY, cilt.77, sa.5, ss.2337-2344, 2012 (SCI İndekslerine Giren Dergi)

XLVII. **Thermal Rearrangements of 1-Ethynyl-2-methylcyclopropane: A Computational Study**
Bozkaya U., ÖZKAN İ.
JOURNAL OF PHYSICAL CHEMISTRY A, cilt.116, sa.12, ss.3274-3281, 2012 (SCI İndekslerine Giren Dergi)

XLVIII. **Potential Energy Surfaces for Rearrangements of Berson Trimethylenemethanes**
Bozkaya U., ÖZKAN İ.
JOURNAL OF PHYSICAL CHEMISTRY A, cilt.116, sa.9, ss.2309-2321, 2012 (SCI İndekslerine Giren Dergi)

XLIX. **Thermal denitrogenation of 7-isopropylidene-2,3-diaza-norbornene: formation of substituted 3-methylene-(1,4)-pentadienes**
Bozkaya U., ÖZKAN İ.
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, cilt.14, sa.41, ss.14282-14292, 2012 (SCI İndekslerine Giren Dergi)

L. **Dihydroxylation of olefins catalyzed by zeolite-confined osmium(0) nanoclusters: an efficient and reusable method for the preparation of 1,2-cis-diols**
Metin O., Alp N. A. , Akbayrak S., Bicer A., GÜLTEKİN M. S. , ÖZKAR S., Bozkaya U.
GREEN CHEMISTRY, cilt.14, sa.5, ss.1488-1492, 2012 (SCI İndekslerine Giren Dergi)

LI. **Orbital-optimized third-order Moller-Plesset perturbation theory and its spin-component and spin-opposite scaled variants: Application to symmetry breaking problems**
Bozkaya U.
JOURNAL OF CHEMICAL PHYSICS, cilt.135, sa.22, 2011 (SCI İndekslerine Giren Dergi)

LII. **Quadratically convergent algorithm for orbital optimization in the orbital-optimized coupled-cluster doubles method and in orbital-optimized second-order Moller-Plesset perturbation theory**
Bozkaya U., Turney J. M. , Yamaguchi Y., Schaefer H. F. , Sherrill C. D.
JOURNAL OF CHEMICAL PHYSICS, cilt.135, sa.10, 2011 (SCI İndekslerine Giren Dergi)

LIII. **The barrier height, unimolecular rate constant, and lifetime for the dissociation of HN2**
Bozkaya U., Turney J. M. , Yamaguchi Y., Schaefer H. F.
JOURNAL OF CHEMICAL PHYSICS, cilt.132, sa.6, 2010 (SCI İndekslerine Giren Dergi)

LIV. **The ten chemically transparent dinitronaphthalene isomers and their radical anions**
Bozkaya U., Schaefer H. F.
MOLECULAR PHYSICS, cilt.108, ss.2491-2509, 2010 (SCI İndekslerine Giren Dergi)

LV. **Network structure and swelling behavior of poly(acrylamide/crotonic acid) hydrogels in aqueous salt solutions**
Caykara T., Bozkaya U., Kantoglu O.
JOURNAL OF POLYMER SCIENCE PART B-POLYMER PHYSICS, cilt.41, sa.14, ss.1656-1664, 2003 (SCI İndekslerine Giren Dergi)

Desteklenen Projeler

BOZKAYA U., Ünal A., Yükseköğretim Kurumları Destekli Proje, Optimize Orbitalli İkili Uyarılmış Çiftleşmiş Küme Teorisinin Enerji ve Analitik Gradient İfadelerinin Modern Tensör Ayrıştırma Yöntemleriyle Formülasyonu Etkin Programlanması ve Açık Kabuklu Kimyasal Sistemlere Uygulamaları, 2016 - 2018
BOZKAYA U., Yükseköğretim Kurumları Destekli Proje, Geçiş Metali Komplekslerinin Moleküler Özelliklerinin ve Elektronik Yapılarının Yüksek Seviyeli Elektron Korelasyon Yöntemleriyle Araştırılması, 2016 - 2017

Atıflar

Toplam Atıf Sayısı (WOS):1257
h-indeksi (WOS):20