Prof. UĞUR BOZKAYA

Personal Information

Email: ugur.bozkaya@hacettepe.edu.tr
Web: https://avesis.hacettepe.edu.tr/ugur.bozkaya

Education Information

Doctorate, Middle East Technical University, Graduate School Of Natural And Applied Sciences, Chemistry, Turkey 2004 - 2011
Undergraduate, Gazi Üniversitesi, Fen-Edebiyat Fakültesi, Kimya Bölümü, Turkey 1999 - 2003

Foreign Languages

English, C1 Advanced

Research Areas

Chemistry, Physical Chemistry, Computational Chemistry, Quantum Mechanics, Natural Sciences

Academic Titles / Tasks

Professor, Hacettepe University, Fen Fakültesi, Kimya Bölümü, 2020 - Continues
Associate Professor, Hacettepe University, Fen Fakültesi, Kimya Bölümü, 2015 - 2020
Associate Professor, Atatürk Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2014 - 2015
Assistant Professor, Atatürk Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2011 - 2014

Academic and Administrative Experience

Atatürk Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2012 - 2014
Atatürk Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2013 - 2013

Advising Theses

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

Articles Published in Journals That Entered SCI, SSCI and AHCI Indexes

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 (Journal Indexed in SCI)

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 (Journal Indexed in SCI)

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, vol.153, no.24, 2020 (Journal Indexed in SCI)

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, vol.5, no.42, pp.13387-13396, 2020 (Journal Indexed in SCI)

V. **Computational Study for the Reaction Mechanism of N-Hydroxyphthalimide-Catalyzed Oxidative Cleavage of Alkenes**
EŞSİZ S., BOZKAYA U.
JOURNAL OF ORGANIC CHEMISTRY, vol.85, no.15, pp.10136-10142, 2020 (Journal Indexed in SCI)

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, vol.124, no.34, pp.6889-6898, 2020 (Journal Indexed in SCI)

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, vol.152, no.18, 2020 (Journal Indexed in SCI)

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, vol.120, no.7, 2020 (Journal Indexed in SCI)

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, vol.152, no.12, 2020 (Journal Indexed in SCI)

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, vol.41, no.8, 2020 (Journal Indexed in SCI)

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, vol.31, no.2, pp.441-449, 2020 (Journal Indexed in SCI)

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, vol.15, no.8, pp.4415-4429, 2019 (Journal Indexed in SCI)

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, vol.15, pp.931-936, 2019 (Journal Indexed in SCI)

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, vol.21, no.2, pp.554-558, 2019 (Journal Indexed in SCI)

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, vol.122, no.17, pp.4375-4380, 2018 (Journal Indexed in SCI)

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, vol.39, no.7, pp.351-360, 2018 (Journal Indexed in SCI)

XVII. **Anionic water pentamer and hexamer clusters: An extensive study of structures and energetics**
ÜNAL A., BOZKAYA U.
JOURNAL OF CHEMICAL PHYSICS, vol.148, no.12, 2018 (Journal Indexed in SCI)

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, vol.121, no.34, pp.6500-6509, 2017 (Journal Indexed in SCI)

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, vol.13, no.7, pp.3185-3197, 2017 (Journal Indexed in SCI)

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, vol.58, no.30, pp.2981-2985, 2017 (Journal Indexed in SCI)

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, vol.147, no.4, 2017 (Journal Indexed in SCI)

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, vol.17, no.13, pp.2056-2065, 2016 (Journal Indexed in SCI)

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, vol.144, no.17, 2016 (Journal Indexed in SCI)

XXIV. **Orbital-optimized linearized coupled-cluster doubles with density-fitting and Cholesky decomposition approximations: an efficient implementation**
BOZKAYA U.
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol.18, no.16, pp.11362-11373, 2016 (Journal Indexed in SCI)

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, vol.144, no.14, 2016 (Journal Indexed in SCI)

XXVI. **Orbital-Optimized MP3 and MP2.5 with Density-Fitting and Cholesky Decomposition Approximations**
BOZKAYA U.
JOURNAL OF CHEMICAL THEORY AND COMPUTATION, vol.12, no.3, pp.1179-1188, 2016 (Journal Indexed in SCI)

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, vol.14, no.31, pp.7490-7494, 2016 (Journal Indexed in SCI)

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, vol.37, no.3, pp.345-353, 2016 (Journal Indexed in SCI)

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, vol.11, no.4, pp.1564-1573, 2015 (Journal Indexed in SCI)

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, vol.141, no.20, 2014 (Journal Indexed in SCI)

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, vol.10, no.10, pp.4389-4399, 2014 (Journal Indexed in SCI)

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, vol.141, no.12, 2014 (Journal Indexed in SCI)

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, vol.10, no.6, pp.2371-2378, 2014 (Journal Indexed in SCI)

XXXIV. **Accurate Electron Affinities from the Extended Koopmans' Theorem Based on Orbital-Optimized Methods**
Bozkaya U.
JOURNAL OF CHEMICAL THEORY AND COMPUTATION, vol.10, no.5, pp.2041-2048, 2014 (Journal Indexed in SCI)

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, vol.35, no.14, pp.1073-1081, 2014 (Journal Indexed in SCI)

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, vol.9, no.11, pp.4679-4683, 2013 (Journal Indexed in SCI)

XXXVII. **The extended Koopmans' theorem for orbital-optimized methods: Accurate computation of ionization potentials**
Bozkaya U.
JOURNAL OF CHEMICAL PHYSICS, vol.139, no.15, 2013 (Journal Indexed in SCI)

XXXVIII. **Analytic energy gradients for the orbital-optimized third-order Moller-Plesset perturbation theory**
Bozkaya U.
JOURNAL OF CHEMICAL PHYSICS, vol.139, no.10, 2013 (Journal Indexed in SCI)

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, vol.139, no.5, 2013 (Journal Indexed in SCI)

XL. **Analytic energy gradients for the orbital-optimized second-order Moller-Plesset perturbation theory**
Bozkaya U., Sherrill C. D.

JOURNAL OF CHEMICAL PHYSICS, vol.138, no.18, 2013 (Journal Indexed in SCI)

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, vol.9, no.3, pp.1452-1460, 2013 (Journal Indexed in SCI)

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, vol.3, no.36, pp.15866-15874, 2013 (Journal Indexed in SCI)

XLIII. **Thermal Aromatizations of 2-Vinylmethylenecyclopropane and 3-Vinylcyclobutene**
Bozkaya U., ÖZKAN İ.
JOURNAL OF ORGANIC CHEMISTRY, vol.77, no.13, pp.5714-5723, 2012 (Journal Indexed in SCI)

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, vol.136, no.20, 2012 (Journal Indexed in SCI)

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, vol.136, no.16, 2012 (Journal Indexed in SCI)

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, vol.77, no.5, pp.2337-2344, 2012 (Journal Indexed in SCI)

XLVII. **Thermal Rearrangements of 1-Ethynyl-2-methylcyclopropane: A Computational Study**
Bozkaya U., ÖZKAN İ.
JOURNAL OF PHYSICAL CHEMISTRY A, vol.116, no.12, pp.3274-3281, 2012 (Journal Indexed in SCI)

XLVIII. **Potential Energy Surfaces for Rearrangements of Berson Trimethylenemethanes**
Bozkaya U., ÖZKAN İ.
JOURNAL OF PHYSICAL CHEMISTRY A, vol.116, no.9, pp.2309-2321, 2012 (Journal Indexed in SCI)

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, vol.14, no.41, pp.14282-14292, 2012 (Journal Indexed in SCI)

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, vol.14, no.5, pp.1488-1492, 2012 (Journal Indexed in SCI)

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, vol.135, no.22, 2011 (Journal Indexed in SCI)

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, vol.135, no.10, 2011 (Journal Indexed in SCI)

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, vol.132, no.6, 2010 (Journal Indexed in SCI)

LIV. **The ten chemically transparent dinitronaphthalene isomers and their radical anions**

Bozkaya U., Schaefer H. F.
MOLECULAR PHYSICS, vol.108, pp.2491-2509, 2010 (Journal Indexed in SCI)

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, vol.41, no.14, pp.1656-1664, 2003 (Journal Indexed in SCI)

Supported Projects

BOZKAYA U., Ünal A., Project Supported by Higher Education Institutions, 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., Project Supported by Higher Education Institutions, Geçiş Metali Komplekslerinin Moleküler Özelliklerinin ve Elektronik Yapılarının Yüksek Seviyeli Elektron Korelasyon Yöntemleriyle Araştırılması, 2016 - 2017

Citations

Total Citations (WOS):1257
h-index (WOS):20