Prof. UĞUR BOZKAYA

Personal Information

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Education Information

Doctorate, Middle East Technical University, Graduate School Of Natural And Applied Sciences, Chemistry, Turkey 2004 - 2011
Under Graduate, 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

Professional Experience

Deputy Head of Department, Atatürk Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2012 - 2014
Mevlana Exchange Program Coordinator, 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, Post Graduate, E.SOYDAŞ(Student), 2015

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

I. **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, pp.6889-6898, 2020 (Journal Indexed in SCI)

II. **Computational Study for the Reaction Mechanism of N-Hydroxyphthalimide-Catalyzed Oxidative Cleavage of Alkenes**
EŞSİZ S., BOZKAYA U.
JOURNAL OF ORGANIC CHEMISTRY, vol.85, pp.10136-10142, 2020 (Journal Indexed in SCI)

III. **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, 2020 (Journal Indexed in SCI)

IV. **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, 2020 (Journal Indexed in SCI)

V. **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, 2020 (Journal Indexed in SCI)

VI. **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, 2020 (Journal Indexed in SCI)

VII. **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, pp.441-449, 2020 (Journal Indexed in SCI)

VIII. **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, pp.4415-4429, 2019 (Journal Indexed in SCI)

IX. **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)

X. **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, pp.554-558, 2019 (Journal Indexed in SCI)

XI. **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, pp.4375-4380, 2018 (Journal Indexed in SCI)

XII. **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, pp.351-360, 2018 (Journal Indexed in SCI)

XIII. **Anionic water pentamer and hexamer clusters: An extensive study of structures and energetics**
ÜNAL A., BOZKAYA U.
JOURNAL OF CHEMICAL PHYSICS, vol.148, 2018 (Journal Indexed in SCI)

XIV. **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, pp.6500-6509, 2017 (Journal Indexed in SCI)

XV. **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, pp.3185-3197, 2017 (Journal Indexed in SCI)

XVI. **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, 2017 (Journal Indexed in SCI)

XVII. **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, pp.2981-2985, 2017 (Journal Indexed in SCI)

XVIII. **Charge-Transfer Complex of p-Aminodiphenylamine with Maleic Anhydride: Spectroscopic, Electrochemical, and Physical Properties**
KARACA E., Can H. K. , BOZKAYA U., Pekmez N. O.
CHEMPHYSCHEM, vol.17, pp.2056-2065, 2016 (Journal Indexed in SCI)

XIX. **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, 2016 (Journal Indexed in SCI)

XX. **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, 2016 (Journal Indexed in SCI)

XXI. **Orbital-optimized linearized coupled-cluster doubles with density-fitting and Cholesky decomposition approximations: an efficient implementation**
BOZKAYA U.
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol.18, pp.11362-11373, 2016 (Journal Indexed in SCI)

XXII. **Orbital-Optimized MP3 and MP2.5 with Density-Fitting and Cholesky Decomposition Approximations**
BOZKAYA U.
JOURNAL OF CHEMICAL THEORY AND COMPUTATION, vol.12, pp.1179-1188, 2016 (Journal Indexed in SCI)

XXIII. **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, pp.7490-7494, 2016 (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):578
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