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Kişisel Bilgiler

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Eğitim Bilgileri

Bütünleşik Doktora, Orta Doğu Teknik Üniversitesi, Fen Bilimleri Enstitüsü, Kimya, Türkiye 2004 - 2011
Lisans, Gazi Üniversitesi, Fen-Edebiyat Fakültesi, Kimya Bölümü, Türkiye 1999 - 2003

Yabancı Diller

İngilizce, C1 İleri

Araştırma Alanları

Kimya, Fizikokimya, Hesapsal Kimya, Kuantum Mekaniği, Temel Bilimler

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
Yrd. Doç. Dr., Atatürk Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2011 - 2014

Akademik İdari Deneyim

Atatürk Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2012 - 2014
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. **Linear-Scaling Systematic Molecular Fragmentation Approach for Perturbation Theory and Coupled-Cluster Methods**
Bozkaya U., Ermis B.
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II. **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**
GÜNDOĞDU Ö., Atalay A., Celebioglu N., ANIL B., ŞAHİN E., Sanli-Mohamed G., BOZKAYA U., KARA Y.
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III. **Accurate property prediction by second order perturbation theory: The REMP and OO-REMP hybrids**
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IV. **Bay- and peri-functionalized donor-acceptor perylene monoimides via nitration and nucleophilic substitution/reduction pathway**
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V. **Efficient Implementation of Equation-of-Motion Coupled-Cluster Singles and Doubles Method with the Density-Fitting Approximation: An Enhanced Algorithm for the Particle-Particle Ladder Term**
ÜNAL A., BOZKAYA U.
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VI. **Efficient and regioselective synthesis of dihydroxy-substituted 2-aminocyclooctane-1-carboxylic acid and its bicyclic derivatives**
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VII. **MacroQC 1.0: An electronic structure theory software for large-scale applications**
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JOURNAL OF CHEMICAL PHYSICS, cilt.156, sa.4, 2022 (SCI-Expanded)

VIII. **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, cilt.19, ss.9483-9490, 2021 (SCI-Expanded)

IX. **Efficient implementations of the symmetric and asymmetric triple excitation corrections for the orbital-optimized coupled-cluster doubles method with the density-fitting approximation**
Alagoz Y., ÜNAL A., BOZKAYA U.
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X. **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, cilt.121, sa.11, 2021 (SCI-Expanded)

XI. **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-Expanded)

XII. **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-Expanded)

XIII. **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.
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XIV. **Computational Study for the Reaction Mechanism of N-Hydroxyphthalimide-Catalyzed Oxidative Cleavage of Alkenes**
EŞSİZ S., BOZKAYA U.
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XV. **PSI4 1.4: Open-source software for high-throughput quantum chemistry**
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XVI. **Ionized water clusters (H2O)(n)(+), n=2 to 6: A high-accuracy study of structures and energetics**
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XVII. **State-of-the-art computations of dipole moments using analytic gradients of high-level density-fitted coupled-cluster methods with focal-point approximations**
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XVIII. **Efficient and automated computation of accurate molecular geometries using focal-point approximations to large-basis coupled-cluster theory**
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XIX. **Conformational Characterization of Polyelectrolyte Oligomers and Their Noncovalent Complexes Using Ion Mobility-Mass Spectrometry**
ATAKAY M., Aksakal F., BOZKAYA U., SALİH B., Wesdemiotis C.
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XX. **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?**
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XXI. **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**
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XXII. **Aza-Nazarov Cyclization Reactions via Anion Exchange Catalysis**
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XXIII. **State-of-the-Art Computations of Vertical Ionization Potentials with the Extended Koopmans' Theorem Integrated with the CCSD(T) Method**
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XXIV. **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-Expanded)

XXV. **Analytic Energy Gradients for Orbital-Optimized MP3 and MP2.5 with the Density-Fitting Approximation: An Efficient Implementation**
BOZKAYA U.
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XXVI. **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-Expanded)

XXVII. **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-Expanded)

XXVIII. **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-Expanded)

XXIX. **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-Expanded)

XXX. **Charge-Transfer Complex of p-Aminodiphenylamine with Maleic Anhydride: Spectroscopic, Electrochemical, and Physical Properties**
KARACA E., Can H., BOZKAYA U., Pekmez N.
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XXXI. **Analytic energy gradients for the coupled-cluster singles and doubles method with the density-fitting approximation**
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XXXII. **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-Expanded)

XXXIII. **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-Expanded)

XXXIV. **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-Expanded)

XXXV. **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-Expanded)

XXXVI. **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.
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XXXVII. **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.
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XXXVIII. **Orbital-optimized MP2.5 and its analytic gradients: Approaching CCSD(T) quality for noncovalent interactions**
Bozkaya U., Sherrill C. D.
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XXXIX. **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-Expanded)

XL. **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-Expanded)

XLI. **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-Expanded)

XLII. **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-Expanded)

XLIII. **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-Expanded)

XLIV. **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-Expanded)

XLV. **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-Expanded)

XLVI. **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-Expanded)

XLVII. **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-Expanded)

XLVIII. **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-Expanded)

XLIX. **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-Expanded)

L. **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-Expanded)

LI. **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-Expanded)

LII. **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-Expanded)

LIII. **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-Expanded)

LIV. **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-Expanded)

LV. **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-Expanded)

LVI. **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.
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LVII. **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-Expanded)

LVIII. **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-Expanded)

LIX. **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-Expanded)

LX. **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-Expanded)

LXI. **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-Expanded)

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

LXIII. **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-Expanded)

Hakemli Kongre / Sempozyum Bildiri Kitaplarında Yer Alan Yayınlar

I. **Assessment of the Density-Fitted Equation-of-Motion Coupled-Cluster Singles and Doubles Method for Excitation Energies**
Bozkaya T., ÜNAL A., BOZKAYA U.
25th International Workshop on Quantum Systems in Chemistry, Physics and Biology (QSCP 2022), Torun, Polonya, 19 Haziran 2022

II. **Equation-of-Motion Orbital-Optimized Second-Order Perturbation Theory with The Density-Fitting**

Approximation
ÜNAL A., BOZKAYA U.
13th Chemical Physics Congress, Elazığ, Türkiye, 15 - 16 Ekim 2020

III. **State-of-the-Art Computations of Vertical Ionization Potentials with the Extended Koopmans**
ÜNAL A., BOZKAYA U.
12th Chemical Physics Congress, Safranbolu, Safranbolu, Türkiye, 12 - 13 Ekim 2018

IV. **Anyonik Su Kümelerinin Yapıları ve Enerjilerinin Kuantum Kimyasal Yöntemlerle Yüksek Doğrulukta Hesaplanması**
ÜNAL A., BOZKAYA U.
3. Hesaplamalı Kimya Kongresi, Ankara, Türkiye, 12 - 14 Ekim 2017

V. **Anyonik Su Kümelerinin Denge Geometrilerinin, Bağlanma ve Dikey Elektron Koparılma Enerjilerinin Kuantum Kimyasal Yöntemlerle Yüksek Doğrulukta Hesaplanması**
ÜNAL A., BOZKAYA U.
6. Fiziksel Kimya Kongresi, Zonguldak, Türkiye, 15 Mayıs 2017 - 18 Nisan 2024

Desteklenen Projeler

Bozkaya U., TÜBİTAK - AB COST Projesi , Yüksek Seviyeli Coupled-Cluster Yöntemlerini Temel Alan Yüksek Doğruluktaki Ab Initio Moleküler Dinamik Simülasyon Yöntemlerinin Geliştirilmesi ve Büyük Ölçekli Moleküler İyonik Kümelerin Simülasyonlarına Uygulanması, 2020 - 2023
Bozkaya U., TÜBİTAK Projesi, Yüksek Seviyeli Bağlanmış Küme ve Pertürbasyon Teorisi Yöntemleri için Hareket Denklemi Yaklaşımının Yoğunluk Fit Edilmesi ve Dondurulmuş Doğal Orbitaller Teknikleriyle Geliştirilmesi, Etkin Programlanması ve Zorlu Kimyasal Sistemlere Uygulanması, 2019 - 2022
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

Metrikler

Yayın: 70
Atıf (WoS): 1293
Atıf (Scopus): 743
H-İndeks (WoS): 20
H-İndeks (Scopus): 19

Akademi Dışı Deneyim

Georgia Institue of Technology
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