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Kişisel Bilgiler

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ScopusID: 57201417805

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Eğitim Bilgileri

Doktora, Hacettepe Üniversitesi, Fen Bilimleri Enstitüsü, Kimya A.B.D., Türkiye 2017 - 2023

Yüksek Lisans, Hacettepe Üniversitesi, Fen Bilimleri Enstitüsü, Kimya A.B.D., Türkiye 2013 - 2017

Lisans, Hacettepe Üniversitesi, Fen Fakültesi, Kimya Bölümü, Türkiye 2008 - 2013

Araştırma Alanları

Kimya

Akademik Unvanlar / Görevler

Öğretim Görevlisi Dr., Hacettepe Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2019 - Devam Ediyor

SCI, SSCI ve AHCI İndekslerine Giren Dergilerde Yayınlanan Makaleler

- I. **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.
JOURNAL OF CHEMICAL THEORY AND COMPUTATION, cilt.18, sa.3, ss.1489-1500, 2022 (SCI-Expanded)
- II. **MacroQC 1.0: An electronic structure theory software for large-scale applications**
BOZKAYA U., Ermis B., Alagoz Y., ÜNAL A., Uyar A. K.
JOURNAL OF CHEMICAL PHYSICS, cilt.156, sa.4, 2022 (SCI-Expanded)
- III. **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.
JOURNAL OF CHEMICAL PHYSICS, cilt.155, sa.11, 2021 (SCI-Expanded)
- IV. **Anharmonic force field from coupled-cluster methods and accurate computation of infrared spectra**
Ermis B., Ünal A., Soydaş E., Bozkaya U.
ADVANCES IN QUANTUM CHEMISTRY, cilt.83, ss.139-153, 2021 (SCI-Expanded)
- V. **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)

- 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-Expanded)

- VII. **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-Expanded)

- VIII. **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-Expanded)

- IX. **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-Expanded)

- X. **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)

Metrikler

Yayın: 10

Atıf (WoS): 37

Atıf (Scopus): 53

H-İndeks (WoS): 4

H-İndeks (Scopus): 4