Lect. PhD ASLI ÜNAL

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Education Information

Doctorate, Hacettepe University, Fen Bilimleri Enstitüsü, Kimya A.B.D., Turkey 2017 - 2023
Postgraduate, Hacettepe University, Fen Bilimleri Enstitüsü, Kimya A.B.D., Turkey 2013 - 2017
Undergraduate, Hacettepe University, Fen Fakültesi, Kimya Bölümü, Turkey 2008 - 2013

Research Areas

Chemistry

Academic Titles / Tasks

Lecturer PhD, Hacettepe University, Fen Fakültesi, Kimya Bölümü, 2019 - Continues

Published journal articles indexed by SCI, SSCI, and AHCI

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, vol.18, no.3, pp.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, vol.156, no.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, vol.155, no.11, 2021 (SCI-Expanded)

IV. **Anharmonic force field from coupled-cluster methods and accurate computation of infrared spectra**
Ermiş B., Ünal A., Soydaş E., Bozkaya U.
ADVANCES IN QUANTUM CHEMISTRY, vol.83, pp.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, vol.153, no.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, vol.124, no.34, pp.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, vol.120, no.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, vol.15, pp.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, vol.122, no.17, pp.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, vol.148, no.12, 2018 (SCI-Expanded)

Metrics

Publication: 10
Citation (WoS): 37
Citation (Scopus): 53
H-Index (WoS): 4
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