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Kişisel Bilgiler

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Eğitim Bilgileri

Post Doktora, Kansas State University, Amerika Birleşik Devletleri 2016 - 2019

Doktora, University of Delaware, Kimya bölümü, Amerika Birleşik Devletleri 2010 - 2016

Yüksek Lisans, İhsan Doğramacı Bilkent Üniversitesi, Fen Fakültesi, Kimya Bölümü, Türkiye 2007 - 2009

Lisans, İhsan Doğramacı Bilkent Üniversitesi, Fen Fakültesi, Kimya Bölümü, Türkiye 2002 - 2007

Araştırma Alanları

Hesapsal Kimya, Kuantum Mekaniği, Spektroskopi, Nanokümelere

SCI, SSCI ve AHCI İndekslerine Giren Dergilerde Yayınlanan Makaleler

- I. **Understanding the Effect of Symmetry Breaking on Plasmon Coupling from TDDFT**
ALKAN F., Aikens C. M.
JOURNAL OF PHYSICAL CHEMISTRY C, cilt.125, sa.22, ss.12198-12206, 2021 (SCI İndekslerine Giren Dergi)
- II. **TD-DFTB study of optical properties of silver nanoparticle homodimers and heterodimers**
Liu Z., Alkan F., Aikens C. M.
JOURNAL OF CHEMICAL PHYSICS, cilt.153, sa.14, 2020 (SCI İndekslerine Giren Dergi)
- III. **A hybridized local and charge transfer excited state for solution-processed non-doped green electroluminescence based on oligo(p-phenyleneethynylene)**
USTA H., Alimli D., ÖZDEMİR R., Tekin E., ALKAN F., Kacar R., Altas A. G., Dabak S., Gurek A. G., MUTLUGÜN E., et al.
JOURNAL OF MATERIALS CHEMISTRY C, cilt.8, sa.24, ss.8047-8060, 2020 (SCI İndekslerine Giren Dergi)
- IV. **Highly Efficient Deep-Blue Electroluminescence Based on a Solution-Processable A-pi-D-pi-A Oligo(p-phenyleneethynylene) Small Molecule**
USTA H., Alimli D., ÖZDEMİR R., Dabak S., Zorlu Y., ALKAN F., Tekin E., CAN A.
ACS APPLIED MATERIALS & INTERFACES, cilt.11, sa.47, ss.44474-44486, 2019 (SCI İndekslerine Giren Dergi)
- V. **Understanding plasmon coupling in nanoparticle dimers using molecular orbitals and configuration interaction**
ALKAN F., Aikens C. M.
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, cilt.21, sa.41, ss.23065-23075, 2019 (SCI İndekslerine Giren Dergi)
- VI. **Understanding the Effect of Doping on Energetics and Electronic Structure for Au-25, Ag-25, and Au-38 Clusters**
Alkan F., Pandeya P., Aikens C. M.
JOURNAL OF PHYSICAL CHEMISTRY C, cilt.123, sa.14, ss.9516-9527, 2019 (SCI İndekslerine Giren Dergi)
- VII. **[Ag-48(C (CBu)-Bu-t)(20)(CrO4)(7)]: An Atomically Precise Silver Nanocluster Co-protected by Inorganic and Organic Ligands**
Zhang S., Alkan F., Su H., Aikens C. M., Tung C., Sun D.
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, cilt.141, sa.10, ss.4460-4467, 2019 (SCI İndekslerine Giren

Dergi)

- VIII. **Different Silver Nanoparticles in One Crystal: Ag-210((PrPhS)-Pr-i)(71)(Ph3P)(5)Cl and Ag-211((PrPhS)-Pr-i)(71)(Ph3P)(6)Cl**
Liu J., Alkan F., Wang Z., Zhang Z., Kurmoo M., Yan Z., Zhao Q., Aikens C. M., Tung C., Sun D.
ANGEWANDTE CHEMIE-INTERNATIONAL EDITION, cilt.58, sa.1, ss.195-199, 2019 (SCI İndekslerine Giren Dergi)
- IX. **Spin-orbit effects on the Te-125 magnetic-shielding tensor: A cluster-based ZORA/DFT investigation**
Alkan F., Dybowski C.
SOLID STATE NUCLEAR MAGNETIC RESONANCE, cilt.95, ss.6-11, 2018 (SCI İndekslerine Giren Dergi)
- X. **TD-DFT and TD-DFTB Investigation of the Optical Properties and Electronic Structure of Silver Nanorods and Nanorod Dimers**
Alkan F., Aikens C. M.
JOURNAL OF PHYSICAL CHEMISTRY C, cilt.122, sa.41, ss.23639-23650, 2018 (SCI İndekslerine Giren Dergi)
- XI. **Relativistic DFT investigation of electronic structure effects arising from doping the Au-25 nanocluster with transition metals**
Alkan F., Munoz-Castro A., Aikens C. M.
NANOSCALE, cilt.9, sa.41, ss.15825-15834, 2017 (SCI İndekslerine Giren Dergi)
- XII. **Role of Exact Exchange and Relativistic Approximations in Calculating F-19 Magnetic Shielding in Solids Using a Cluster Ansatz**
Alkan F., Holmes S. T., Dybowski C.
JOURNAL OF CHEMICAL THEORY AND COMPUTATION, cilt.13, sa.10, ss.4741-4752, 2017 (SCI İndekslerine Giren Dergi)
- XIII. **Analysis of the Bond-Valence Method for Calculating Si-29 and P-31 Magnetic Shielding in Covalent Network Solids**
Holmes S. T., Alkan F., Iuliucci R. J., Mueller K. T., Dybowski C.
JOURNAL OF COMPUTATIONAL CHEMISTRY, cilt.37, sa.18, ss.1704-1710, 2016 (SCI İndekslerine Giren Dergi)
- XIV. **Spin-orbit effects on the Sn-119 magnetic-shielding tensor in solids: a ZORA/DFT investigation**
Alkan F., Holmes S. T., Iuliucci R. J., Mueller K. T., Dybowski C.
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, cilt.18, sa.28, ss.18914-18922, 2016 (SCI İndekslerine Giren Dergi)
- XV. **Ion pairing in H2O and D2O solutions of lead nitrate, as determined with Pb-207 NMR spectroscopy**
Alkan F., Small T., Bai S., Dominowski A., Dybowski C.
JOURNAL OF STRUCTURAL CHEMISTRY, cilt.57, sa.2, ss.369-375, 2016 (SCI İndekslerine Giren Dergi)
- XVI. **Effect of Co-Ordination Chemistry and Oxidation State on the Pb-207 Magnetic-Shielding Tensor: A DFT/ZORA Investigation**
Alkan F., Dybowski C.
JOURNAL OF PHYSICAL CHEMISTRY A, cilt.120, sa.1, ss.161-168, 2016 (SCI İndekslerine Giren Dergi)
- XVII. **Chemical-shift tensors of heavy nuclei in network solids: a DFT/ZORA investigation of Pb-207 chemical-shift tensors using the bond-valence method**
Alkan F., Dybowski C.
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, cilt.17, sa.38, ss.25014-25026, 2015 (SCI İndekslerine Giren Dergi)
- XVIII. **Pb-207 and Sn-119 Solid-State NMR and Relativistic Density Functional Theory Studies of the Historic Pigment Lead-Tin Yellow Type I and Its Reactivity in Oil Paintings**
Catalano J., Murphy A., Yao Y., Alkan F., Zurnbulyadis N., Centeno S. A., Dybowski C.
JOURNAL OF PHYSICAL CHEMISTRY A, cilt.118, sa.36, ss.7952-7958, 2014 (SCI İndekslerine Giren Dergi)
- XIX. **Calculation of chemical-shift tensors of heavy nuclei: a DFT/ZORA investigation of Hg-199 chemical-shift tensors in solids, and the effects of cluster size and electronic-state approximations**
Alkan F., Dybowski C.
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, cilt.16, sa.27, ss.14298-14308, 2014 (SCI İndekslerine Giren Dergi)
- XX. **A Combined NMR and DFT Study of Narrow Gap Semiconductors: The Case of PbTe**
Taylor R. E., Alkan F., Koumoulis D., Lake M. P., King D., Dybowski C., Bouchard L.
JOURNAL OF PHYSICAL CHEMISTRY C, cilt.117, sa.17, ss.8959-8967, 2013 (SCI İndekslerine Giren Dergi)
- XXI. **Theoretical investigation of excited states of oligothiophene anions**

Alkan F., Salzner U.

JOURNAL OF PHYSICAL CHEMISTRY A, cilt.112, sa.27, ss.6053-6058, 2008 (SCI İndekslerine Giren Dergi)

Hakemli Kongre / Sempozyum Bildiri Kitaplarında Yer Alan Yayınlar

I. **TD-DFTB investigation of electronic structure and optical properties of silver nanorods and nanorod dimers**

Alkan F., Aikens C.

255th National Meeting and Exposition of the American-Chemical-Society (ACS) - Nexus of Food, Energy, and Water, Louisiana, Amerika Birleşik Devletleri, 18 - 22 Mart 2018, cilt.255

II. **Theoretical investigation of the electronic structure and stability for doped Au₂₅ clusters**

Alkan F., Munoz Castro A., Aikens C.

255th National Meeting and Exposition of the American-Chemical-Society (ACS) - Nexus of Food, Energy, and Water, Louisiana, Amerika Birleşik Devletleri, 18 - 22 Mart 2018, cilt.255

Bilimsel Hakemlikler

JOURNAL OF PHYSICAL CHEMISTRY C, SCI Kapsamındaki Dergi, Haziran 2021

INORGANIC CHEMISTRY, SCI Kapsamındaki Dergi, Mayıs 2021

PHYSICAL CHEMISTRY CHEMICAL PHYSICS, SCI Kapsamındaki Dergi, Aralık 2020

JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, SCI Kapsamındaki Dergi, Mayıs 2019

Atıflar

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