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Personal Information

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Education Information

Post Doctorate, Kansas State University, United States Of America 2016 - 2019

Doctorate, University of Delaware, arts and sciences, chemistry, United States Of America 2010 - 2016

Postgraduate, İhsan Doğramacı Bilkent Üniversitesi, Faculty Of Science, Department Of Chemistry, Turkey 2007 - 2009

Undergraduate, İhsan Doğramacı Bilkent Üniversitesi, Faculty Of Science, Department Of Chemistry, Turkey 2002 - 2007

Research Areas

Computational Chemistry, Quantum Mechanics, Spectroscopy, nanoclusters

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

- I. **Understanding the Effect of Symmetry Breaking on Plasmon Coupling from TDDFT**
ALKAN F., Aikens C. M.
JOURNAL OF PHYSICAL CHEMISTRY C, vol.125, no.22, pp.12198-12206, 2021 (Journal Indexed in SCI)
- II. **TD-DFTB study of optical properties of silver nanoparticle homodimers and heterodimers**
Liu Z., Alkan F., Aikens C. M.
JOURNAL OF CHEMICAL PHYSICS, vol.153, no.14, 2020 (Journal Indexed in SCI)
- 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, vol.8, no.24, pp.8047-8060, 2020 (Journal Indexed in SCI)
- 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, vol.11, no.47, pp.44474-44486, 2019 (Journal Indexed in SCI)
- V. **Understanding plasmon coupling in nanoparticle dimers using molecular orbitals and configuration interaction**
ALKAN F., Aikens C. M.
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol.21, no.41, pp.23065-23075, 2019 (Journal Indexed in SCI)
- 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, vol.123, no.14, pp.9516-9527, 2019 (Journal Indexed in SCI)
- 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, vol.141, no.10, pp.4460-4467, 2019 (Journal Indexed in SCI)

- 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, vol.58, no.1, pp.195-199, 2019 (Journal Indexed in SCI)
- 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, vol.95, pp.6-11, 2018 (Journal Indexed in SCI)
- 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, vol.122, no.41, pp.23639-23650, 2018 (Journal Indexed in SCI)
- 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, vol.9, no.41, pp.15825-15834, 2017 (Journal Indexed in SCI)
- 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, vol.13, no.10, pp.4741-4752, 2017 (Journal Indexed in SCI)
- 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., Iulicci R. J. , Mueller K. T. , Dybowski C.
JOURNAL OF COMPUTATIONAL CHEMISTRY, vol.37, no.18, pp.1704-1710, 2016 (Journal Indexed in SCI)
- XIV. **Spin-orbit effects on the Sn-119 magnetic-shielding tensor in solids: a ZORA/DFT investigation**
Alkan F., Holmes S. T. , Iulicci R. J. , Mueller K. T. , Dybowski C.
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol.18, no.28, pp.18914-18922, 2016 (Journal Indexed in SCI)
- 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, vol.57, no.2, pp.369-375, 2016 (Journal Indexed in SCI)
- 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, vol.120, no.1, pp.161-168, 2016 (Journal Indexed in SCI)
- 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, vol.17, no.38, pp.25014-25026, 2015 (Journal Indexed in SCI)
- 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, vol.118, no.36, pp.7952-7958, 2014 (Journal Indexed in SCI)
- 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, vol.16, no.27, pp.14298-14308, 2014 (Journal Indexed in SCI)
- 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, vol.117, no.17, pp.8959-8967, 2013 (Journal Indexed in SCI)
- XXI. **Theoretical investigation of excited states of oligothiophene anions**
Alkan F., Salzner U.
JOURNAL OF PHYSICAL CHEMISTRY A, vol.112, no.27, pp.6053-6058, 2008 (Journal Indexed in SCI)

Refereed Congress / Symposium Publications in Proceedings

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, United States Of America, 18 - 22 March 2018, vol.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, United States Of America, 18 - 22 March 2018, vol.255

Scientific Refereeing

JOURNAL OF PHYSICAL CHEMISTRY C, SCI Journal, June 2021

INORGANIC CHEMISTRY, SCI Journal, May 2021

PHYSICAL CHEMISTRY CHEMICAL PHYSICS, SCI Journal, December 2020

JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, SCI Journal, May 2019

Citations

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