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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, Ihsan Dogramaci Bilkent University, Faculty Of Scıence, Department Of Chemıstry, Turkey 2007 - 2009
Undergraduate, Ihsan Dogramaci Bilkent University, Faculty Of Scıence, Department Of Chemıstry, Turkey 2002 - 2007

Research Areas

Computational Chemistry, Quantum Mechanics, Spectroscopy, nanoclusters

Academic Titles / Tasks

Assistant Professor, Abdullah Gul University, Mühendislik Fakültesi, Nanoteknoloji Mühendisliği, 2019 - Continues

Published journal articles indexed by SCI, SSCI, and AHCI

I. **Theoretical investigation of steric effects on the S1 potential energy surface of o-carborane-anthracene derivatives**
Alkan F.
Turkish Journal of Chemistry, vol.47, no.3, pp.646-655, 2023 (SCI-Expanded)

II. **An Ultrastable 155-Nuclei Silver Nanocluster Protected by Thiacalix[4]arene and Cyclohexanethiol for Photothermal Conversion**
Wang Z., ALKAN F., Aikens C. M., Kurmoo M., Zhang Z., Song K., Tung C., Sun D.
ANGEWANDTE CHEMIE-INTERNATIONAL EDITION, vol.61, no.31, 2022 (SCI-Expanded)

III. **Revisiting the Role of Charge Transfer in the Emission Properties of Carborane-Fluorophore Systems: A TDDFT Investigation**
TAHAOĞLU D., USTA H., ALKAN F.
JOURNAL OF PHYSICAL CHEMISTRY A, vol.126, no.26, pp.4199-4210, 2022 (SCI-Expanded)

IV. **Theoretical investigation of substituent effects on the relative stabilities and electronic structure of [BnXn](2-) clusters**
TAHAOĞLU D., ALKAN F., DURANDURDU M.
JOURNAL OF MOLECULAR MODELING, vol.27, no.12, 2021 (SCI-Expanded)

V. **Understanding and Tailoring Excited State Properties in Solution-Processable Oligo(p-phenyleneethynylene)s: Highly Fluorescent Hybridized Local and Charge Transfer Character via Experiment and Theory**
USTA H., ÇOŞUT B., ALKAN F.
JOURNAL OF PHYSICAL CHEMISTRY B, vol.125, no.42, pp.11717-11731, 2021 (SCI-Expanded)

VI. **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 (SCI-Expanded)

VII. **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 (SCI-Expanded)

VIII. **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 (SCI-Expanded)

IX. **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 (SCI-Expanded)

X. **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 (SCI-Expanded)

XI. **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 (SCI-Expanded)

XII. **[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 (SCI-Expanded)

XIII. **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 (SCI-Expanded)

XIV. **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 (SCI-Expanded)

XV. **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 (SCI-Expanded)

XVI. **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 (SCI-Expanded)

XVII. **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 (SCI-Expanded)

XVIII. **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, vol.37, no.18, pp.1704-1710, 2016 (SCI-Expanded)

XIX. **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, vol.18, no.28, pp.18914-18922, 2016 (SCI-Expanded)

XX. **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 (SCI-Expanded)

XXI. **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 (SCI-Expanded)

XXII. **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 (SCI-Expanded)

XXIII. **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 (SCI-Expanded)

XXIV. **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 (SCI-Expanded)

XXV. **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 (SCI-Expanded)

XXVI. **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 (SCI-Expanded)

Articles Published in Other Journals

I. **External complexation of BODIPYs by CB[7] improves in-cell fluorescence imaging**
Ayhan M. M., Ozcan E., ALKAN F., Cetin M., Un I., Bardelang D., Cosut B.
MATERIALS ADVANCES, vol.3, pp.547-553, 2022 (ESCI)

Refereed Congress / Symposium Publications in Proceedings

I. **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

II. **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

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

Metrics

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