

## Assoc. Prof. ABDULLAH ÖZKANLAR

### Personal Information

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### International Researcher IDs

ORCID: 0000-0003-4634-0468

Yoksis Researcher ID: 219067

### Education Information

Post Doctorate, Max Planck Society, Fritz Haber Institute (Fhi), Theory, Germany 2014 - 2015

Post Doctorate, Washington State University, Faculty Of Science, Physical Chemistry, United States Of America 2010 - 2014

Doctorate, Purdue University, Faculty Of Science, Physics, United States Of America 2003 - 2010

Postgraduate, Bogazici University, Fen Bilimleri, Fizik, Turkey 2001 - 2003

Undergraduate, Bogazici University, Faculty Of Arts And Sciences, Fizik, Turkey 1996 - 2001

### Foreign Languages

English, C1 Advanced

### Dissertations

Doctorate, Spin Dependent Ligand Binding Reactions of Iron-Containing Complexes and Proteins, Purdue University, Faculty Of Science, Physics, 2010

Postgraduate, Representations of  $SL_q(2, \mathbb{R})$  Quantum Groups, Boğaziçi Üniversitesi, Fen Bilimleri, Fizik, 2003

### Research Areas

Basic Sciences, Physics, Atomic and Molecular Physics, Theory of Atoms and Molecules, Interdisciplinary Physics and Related Science and Technology Areas, Physical Chemistry

### Academic Titles / Tasks

Associate Professor, Erciyes University, Fen Fakültesi, Fizik, 2019 - Continues

Assistant Professor, Erciyes University, Fen Fakültesi, Fizik, 2018 - 2019

Assistant Professor, Erciyes University, Fen Fakültesi, Fizik, 2016 - 2018

Lecturer PhD, Kadir Has University, Faculty Of Engineering And Natural Sciences, Biyoinformatik Ve Genetik Bölümü, 2015 - 2016

Research Assistant PhD, Washington State University, Faculty Of Science, Chemistry Department, 2010 - 2014

Research Assistant, Purdue University, Faculty Of Science, Physics Department, 2003 - 2010

Research Assistant, Bogazici University, Fen Edebiyat Fakültesi, Fizik Bölümü, 2001 - 2003

## Academic and Administrative Experience

Head of Department, Erciyes University, Fen Fakültesi, Fizik, 2021 - Continues

## Courses

PHYSICS-II, Undergraduate, 2017 - 2018

Fizik-II, Undergraduate, 2017 - 2018

PHYSICS-I, Undergraduate, 2017 - 2018

Fizik-I, Undergraduate, 2017 - 2018

Kuantum Mekaniği-I, Postgraduate, 2016 - 2017

## Published journal articles indexed by SCI, SSCI, and AHCI

- I. **Intermolecular interactions in binary mixtures of formamide and acetone**  
ÖZKANLAR A.  
Fluid Phase Equilibria, vol.560, 2022 (SCI-Expanded)
- II. **Intermolecular interaction network in liquid acetone**  
ÖZKANLAR A.  
FLUID PHASE EQUILIBRIA, vol.553, 2022 (SCI-Expanded)
- III. **Structure of the Hydrogen-Bond Network in Binary Mixtures of Formamide and Methanol**  
ÖZKANLAR A.  
Journal of Solution Chemistry, vol.50, pp.257-276, 2021 (SCI-Expanded)
- IV. **Structural properties of hydrogen-bond network in liquid formamide-water mixtures**  
ÖZKANLAR A.  
FLUID PHASE EQUILIBRIA, vol.456, pp.98-108, 2018 (SCI-Expanded)
- V. **Towards a unified description of the hydrogen bond network of liquid water: A dynamics based approach**  
Ozkanlar A., ZHOU T., CLARK A. E.  
JOURNAL OF CHEMICAL PHYSICS, vol.141, no.21, 2014 (SCI-Expanded)
- VI. **ChemNetworks: A Complex Network Analysis Tool for Chemical Systems**  
Ozkanlar A., Clark A. E.  
JOURNAL OF COMPUTATIONAL CHEMISTRY, vol.35, no.6, pp.495-505, 2014 (SCI-Expanded)
- VII. **Water Organization and Dynamics on Mineral Surfaces Interrogated by Graph Theoretical Analyses of Intermolecular Chemical Networks**  
Ozkanlar A., Kelley M. P., Clark A. E.  
MINERALS, vol.4, no.1, pp.118-129, 2014 (SCI-Expanded)
- VIII. **Modulation of hydride formation energies in transition metal doped Mg by alteration of spin state**  
Ozkanlar A., Samuels A., Clark A. E.  
CHEMICAL PHYSICS LETTERS, vol.560, pp.10-14, 2013 (SCI-Expanded)
- IX. **Sensitivity of the properties of ruthenium "blue dimer" to method, basis set, and continuum model**  
Ozkanlar A., Clark A. E.  
JOURNAL OF CHEMICAL PHYSICS, vol.136, no.20, 2012 (SCI-Expanded)
- X. **"Covalent Hydration" Reactions in Model Monomeric Ru 2,2 '-Bipyridine Complexes: Thermodynamic Favorability as a Function of Metal Oxidation and Overall Spin States**  
Ozkanlar A., Cape J. L., Hurst J. K., Clark A. E.

## Articles Published in Other Journals

I. **Billiard Physics: Motion of a Cue Ball after Hit by a Cue Stick Horizontally**

ÖZKANLAR A.

The Physics Educator, vol.2, no.1, 2020 (Scopus)

## Refereed Congress / Symposium Publications in Proceedings

I. **Temperature Dependent Structure of Intermolecular Interaction Network in Liquid Formamide**

Özkanlar A., Al-Hadeethi O. J. S.

Turkish Physical Society 38th International Physics Congress, Muğla, Turkey, 31 August - 04 September 2022, vol.04, no.2, pp.19-25

II. **Role of Spin Transitions on the Binding Rate of Peroxynitrite [OONO-] to Iron(III) 5,10,15,20-Tetrakis (N-Methyl-4-Pyridyl) Porphyrin [Fe(III)TMPyP]**

Özkanlar A., Rodriguez J. H.

Turkish Physical Society 38th International Physics Congress, Muğla, Turkey, 31 August - 04 September 2022, pp.56

III. **Hydrogen-Bonding Network of Solvent Water About Cobalt Oxide Water Oxidation Catalysts: Structural and Dynamical Properties**

Özkanlar A.

Turkish Physical Society 33rd International Physics Congress, Muğla, Turkey, 6 - 10 September 2017, pp.243

IV. **Building Water Microstates: A Multilayered Approach**

Özkanlar A.

Turkish Physical Society 33rd International Physics Congress, Muğla, Turkey, 6 - 10 September 2017, pp.223

V. **Implications of Solvent Organization Upon Covalent Hydration of Bipyridine in [(NH<sub>3</sub>)<sub>3</sub>(bpy)Ru=O]<sup>3+</sup>**

Özkanlar A., Clark A. E.

10th Congress on Electronic Structure: Principles and Applications, Castello, Spain, 28 June - 01 July 2016, pp.303-304

VI. **Interfacial chemistry viewed through the lens of network analysis**

CLARK A. E., ÖZKANLAR A., KELLEY M. P.

Goldschmidt Conference 2013, Florence, Italy, 25 - 30 August 2013, pp.893

VII. **Buyer beware: Pitfalls and challenges when studying water oxidation chemistry using DFT**

CLARK A. E., ÖZKANLAR A.

242nd ACS National Meeting & Exposition, Denver, Colorado, United States Of America, 28 August - 01 September 2011, pp.545

VIII. **Water addition reactions in model monomeric Ru 2,2'-bipyridine complexes involving "Covalent Hydration" of bipyridine ligand: Thermodynamic favorability and spectroscopic signatures as a function of metal oxidation and overall spin states**

ÖZKANLAR A., CAPE J. L., HURST J. K., CLARK A. E.

242nd ACS National Meeting & Exposition, Denver, Colorado, United States Of America, 28 August - 01 September 2011, pp.190

IX. **Computational Electronic Structure and Spin Forbidden Reactivity of Iron Tetracarbonyl Complexes**

ÖZKANLAR A., Rodriguez J. H.

42nd Midwest Theoretical Chemistry Conference, West Lafayette, Indiana, United States Of America, 20 - 22 May 2010, pp.24

X. **pH-dependent electronic structure and computed Raman activity of the {FeNO}<sub>6</sub> active site of the**

#### **heme protein nitrophorin-4**

Rodriguez J. H., ÖZKANLAR A., Yue Y., Deligkaris C.

239th ACS National Meeting & Exposition, San Francisco, California, United States Of America, 21 - 25 March 2010, pp.263

XI. **Electronic structure and reactivity of iron tetracarbonyl complexes**

ÖZKANLAR A., Rodriguez J. H.

238th ACS National Meeting, Washington, Dc, United States Of America, 16 - 20 August 2009, pp.118

XII. **Ab-Initio Based Computation of Rate Constants of Spin Forbidden Transitions in (Bio)inorganic Complexes and Metalloproteins**

ÖZKANLAR A., Rodriguez J. H.

2009 APS March Meeting, Pittsburgh, Pennsylvania, United States Of America, 16 March 2009, pp.40

XIII. **Ab-Initio Based Computation of Rate Constants for Spin Forbidden Metalloprotein-Substrate Reactions**

ÖZKANLAR A., Rodriguez J. H.

2007 APS March Meeting, Denver, Colorado, United States Of America, 5 - 09 March 2007

#### **Metrics**

Publication: 24

Citation (WoS): 94

Citation (Scopus): 3

H-Index (WoS): 5

H-Index (Scopus): 1