

## Prof. HAKAN KAYI

### Personal Information

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### International Researcher IDs

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Publons / Web Of Science ResearcherID: C-7300-2009

ScopusID: 22938517300

Yoksis Researcher ID: 17253

### Biography

Dr. Kayı obtained his B.Sc. and M.Sc. degrees in Chemical Engineering from Hacettepe University. He started his Ph.D. studies in the Computer-Chemie-Centrum of the FAU Erlangen-Nürnberg, Germany with the *full scholarship* of Deutsche Forschungsgemeinschaft (DFG), and obtained his Dr. rer. nat. degree in 2009. Then he started to work as a postdoctoral research fellow at the University of Hawaii at Manoa on the *Kuiper Belt Objects* project supported by W.M. Keck Foundation, NASA Astrobiology Institute and University of Hawaii. After successfully completion of the project, he moved to University of Texas at Austin as a postdoctoral research associate in the Institute for Theoretical Chemistry to work on a *pseudo Jahn-Teller effect* related project. He came back to serve his motherland in 2013.

For his research lab, please visit: <http://compchem.ankara.edu.tr/>

### Education Information

Doctorate, Friedrich Alexander Universitat Erlangen Nürnberg, Kimya, Germany 2004 - 2009

Postgraduate, Hacettepe University, Fen Bilimleri Enstitüsü, Kimya Mühendisliği (YI) (Tezli), Turkey 2000 - 2003

Undergraduate, Hacettepe University, Mühendislik Fakültesi, Kimya Mühendisliği Bölümü, Turkey 1995 - 2000

### Foreign Languages

English, C1 Advanced

### Dissertations

Doctorate, Parameterization of the AM1 semiempirical molecular orbital method for the first-row transition metals and other elements, Friedrich Alexander Universitat Erlangen Nürnberg, Kimya, 2009

Postgraduate, Prediction of the lower critical solution temperature of N-isopropylacrylamide-acrylic acid copolymer by an artificial neural network model, Hacettepe University, Fen Bilimleri Enstitüsü, Kimya Mühendisliği A.B.D., 2003

## Research Areas

Chemical Engineering and Technology, Chemistry

## Academic Titles / Tasks

Associate Professor, Ankara University, Mühendislik Fakültesi, Kimya Mühendisliği Bölümü, 2020 - Continues

Assistant Professor, Ankara University, Mühendislik Fakültesi, Kimya Mühendisliği Bölümü, 2018 - 2020

Assistant Professor, Atilim University, Faculty Of Engineering, Department Of Chemistry Engineering And Applied Chemistry, 2013 - 2018

Researcher, The University of Texas at Austin, Institute for Theoretical Chemistry, Chemistry, 2011 - 2013

Researcher, University of Hawaii at Manoa, Chemistry, W.M. Keck Research Laboratory in Astrochemistry, 2010 - 2011

Research Assistant, Friedrich-Alexander-Universitaet Erlangen-Nürnberg, Chemie Und Pharmazie, Computer-Chemie-Centrum, 2004 - 2009

Research Assistant, Hacettepe University, Mühendislik Fakültesi, Kimya Mühendisliği Bölümü, 2001 - 2004

## Academic and Administrative Experience

Assistant Director of the Institute, Ankara University, Fen Bilimleri Enstitüsü, 2020 - 2022

Deputy Head of Department, Ankara University, Mühendislik Fakültesi, Kimya Mühendisliği Bölümü, 2018 - 2019

## Courses

### Doctorate

Kimyasal Hesaplamalar, Doctorate, 2013 - 2014

### Postgraduate

Kimyasal Proses Endüstrileri, Postgraduate, 2017 - 2018, 2016 - 2017, 2014 - 2015

### Undergraduate

HEAT TRANSFER, Undergraduate, 2023 - 2024, 2022 - 2023, 2021 - 2022, 2020 - 2021

KİMYA MÜHENDİSLİĞİ LABORATUVARI I, Undergraduate, 2023 - 2024, 2022 - 2023, 2021 - 2022, 2020 - 2021

CHEMICAL ENGINEERING LAB I, Undergraduate, 2022 - 2023, 2021 - 2022

CHEMICAL ENGINEERING LAB III, Undergraduate, 2022 - 2023, 2021 - 2022

KİMYA MÜHENDİSLİĞİ LABORATUVARI III, Undergraduate, 2022 - 2023, 2020 - 2021, 2019 - 2020

GRADUATION THESIS II, Undergraduate, 2022 - 2023

FLUID MECHANICS, Undergraduate, 2022 - 2023, 2021 - 2022, 2019 - 2020, 2018 - 2019

FLUID MECHANICS, Undergraduate, 2022 - 2023, 2020 - 2021, 2019 - 2020

PROCESS DESIGN I, Undergraduate, 2023 - 2024, 2022 - 2023

PROCESS DESIGN I, Undergraduate, 2022 - 2023

SCIENTIFIC, CULTURAL and SOCIAL ACTIVITIES, Undergraduate, 2022 - 2023

PROCESS DESIGN II, Undergraduate, 2021 - 2022

ARAŞTIRMA TEKNİKLERİ II, Undergraduate, 2021 - 2022, 2020 - 2021, 2019 - 2020

NUMERICAL METHODS, Undergraduate, 2021 - 2022, 2020 - 2021, 2019 - 2020

ARAŞTIRMA TEKNİKLERİ, Undergraduate, 2021 - 2022, 2020 - 2021

GRADUATION THESIS, Undergraduate, 2022 - 2023

INTERNSHIP, Undergraduate, 2022 - 2023

NUMERICAL METHODS, Undergraduate, 2021 - 2022, 2019 - 2020, 2018 - 2019

ARAŞTIRMA TEKNİKLERİ, Undergraduate, 2021 - 2022

INTERNSHIP, Undergraduate, 2021 - 2022

ARAŞTIRMA TEKNİKLERİ I, Undergraduate, 2021 - 2022, 2020 - 2021  
PROCESS DESIGN I, Undergraduate, 2021 - 2022  
KİMYA MÜHENDİSLİĞİ LABORATUVARI III, Undergraduate, 2021 - 2022  
KİMYA MÜHENDİSLİĞİ LABORATUVARI II, Undergraduate, 2020 - 2021  
INTRODUCTION TO CHEMICAL ENGINEERING, Undergraduate, 2021 - 2022, 2020 - 2021, 2019 - 2020, 2018 - 2019  
PROSES TASARIMI I, Undergraduate, 2020 - 2021, 2019 - 2020  
ORIENTATION PROGRAMMING TO THE UNIVERSITY LIFE, Undergraduate, 2019 - 2020  
ISI VE KÜTLE TRANSFERİ, Undergraduate, 2017 - 2018, 2016 - 2017, 2015 - 2016, 2014 - 2015  
KİMYASAL SÜREÇ HESAPLAMALARI, Undergraduate, 2017 - 2018, 2016 - 2017, 2015 - 2016, 2014 - 2015, 2013 - 2014, 2012 - 2013  
ÇEVRE KİRLİLİĞİ, Undergraduate, 2017 - 2018, 2016 - 2017, 2015 - 2016, 2014 - 2015  
MÜHENDİSLİKTE KÜTLE VE ENERJİ DENKLİKLERİ, Undergraduate, 2017 - 2018, 2016 - 2017, 2015 - 2016, 2014 - 2015, 2013 - 2014

## Supervised Theses

Kayi H., Not defined., Doctorate, E.NUR(Student), Continues  
Kayi H., Metal Organic Framework Based Fertilizer Production: MolecularSimulation and Controlled Release Applications, Doctorate, R.TAŞ(Student), Continues  
KAYI H., Benzokalkojendiazol bazı verici-alıcı-verici tipi polimerlerin elektronik bant aralığının yoğunluk fonksiyoneli teorisiyle incelenmesi, Postgraduate, Ö.ÖZKILINÇ(Student), 2021  
KAYI H., Alüminyum yüzeylere uygulanan su bazlı ve solvent bazlı boyaların çevresel etki ve dayanımlarının incelenmesi, Postgraduate, C.KÜÇÜKOĞLU(Student), 2021  
KAYI H., Kalkojen atomlarının kalkojendiazolokinoksalin içeren yarı iletken polimerlerin elektronik bant aralığı üzerindeki etkilerinin kuantum mekanik yöntemlerle incelenmesi, Postgraduate, E.UYANIK(Student), 2021  
KAYI H., Prediction of kinematic viscosity and density of diesel fuel from physical properties by artificial neural networks, Postgraduate, A.ABDULQADER(Student), 2020  
KAYI H., Prediction of chemical oxygen demand from the chemical composition of wastewater by artificial neural networks, Postgraduate, B.AHMED(Student), 2019  
KAYI H., Design of novel platinum and palladium complexes containing pyridyl type ligands for cancer tumor treatment using molecular modeling approach, Doctorate, R.HADI(Student), 2018  
KAYI H., Prediction of the kinematic viscosity of petroleum fractions, Postgraduate, H.AHMED(Student), 2018  
KAYI H., Neural network prediction of flash point of diesel fuel from its chemical composition and physical properties, Postgraduate, Y.MUHSIN(Student), 2017  
KAYI H., Design and optimization of an atmospheric distillation unit in an oil refinery, Postgraduate, K.HUSEIN(Student), 2017  
KAYI H., Modeling and simulation of a vacuum distillation unit in an oil refinery, Postgraduate, A.M.ALI(Student), 2017  
KAYI H., Recovery of silver from silver oxide batteries: A combined experimental and computational study, Postgraduate, A.BUSHRA(Student), 2017  
KAYI H., Theoretical investigation of carbonyl sulfide capture by aqueous diethanolamine solution, Postgraduate, A.MEFTAH(Student), 2017

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

- I. **Effect of chalcogen atoms on the electronic band gaps of the quinoxaline containing donor-acceptor-donor type semiconducting polymers: a systematic DFT investigation**  
Kayi H., Şen E., Özkılınç Ö.  
JOURNAL OF MOLECULAR MODELING, vol.30, pp.1-12, 2024 (SCI-Expanded)
- II. **Ti-substituted organosilica membranes for H<sub>2</sub> sieving: Sol-gel and DFT insights**

KAYI H., Kaya P., Kurt T., Mirza E. S., TOPUZ B.

INTERNATIONAL JOURNAL OF HYDROGEN ENERGY, vol.65, pp.496-504, 2024 (SCI-Expanded)

- III. **Antiproliferative activity of platinum(II) and copper(II) complexes containing novel biquinoxaline ligands**  
El-Beshti H. S., Gercek Z., KAYI H., Yildizhan Y., Cetin Y., Adiguzel Z., Gungor G., Ozalp-Yaman S.  
METALLOMICS, vol.16, no.2, 2024 (SCI-Expanded)
- IV. **Design of a Zr-based metal-organic framework as an efficient fosfomycin carrier: a combined experimental and DFT study**  
Topuz B., Kayi H., Şahin T., Ersoy F. Ş., Günyaktı A., Karakeçili A.  
NEW JOURNAL OF CHEMISTRY, vol.47, no.3, pp.1278-1290, 2023 (SCI-Expanded)
- V. **Anticancer investigation of platinum and copper-based complexes containing quinoxaline ligands**  
El-Beshti H. S., Yildizhan Y., KAYI H., Cetin Y., Adiguzel Z., Gungor-Topcu G., GERÇEK Z., ÖZALP YAMAN Ş.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1250, 2022 (SCI-Expanded)
- VI. **Monodisperse-porous cerium oxide microspheres carrying iridium oxide nanoparticles as a heterogeneous catalyst for water oxidation**  
HAMALOĞLU K. Ö., Tosun R. B., KAYI H., AKKAŞ KAVAKLI P., KAVAKLI C., Tuncel A.  
APPLIED SURFACE SCIENCE, vol.547, 2021 (SCI-Expanded)
- VII. **Monodisperse-porous cerium oxide microspheres as a new support with appreciable catalytic activity for a composite catalyst in benzyl alcohol oxidation**  
HAMALOĞLU K. Ö., Tosun R. B., Ulu S., KAYI H., KAVAKLI C., AKKAŞ KAVAKLI P., Kip C., Tuncel A.  
NEW JOURNAL OF CHEMISTRY, vol.45, no.4, pp.2019-2029, 2021 (SCI-Expanded)
- VIII. **Capture of Carbonyl Sulfide by Organic Liquid Mixtures: A Systematic DFT Investigation**  
Abduesslam M., KAYI H.  
INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH, vol.60, no.3, pp.1366-1374, 2021 (SCI-Expanded)
- IX. **Radical cleavage pathway and DNA docking studies of novel chemotherapeutic platinum agent of 5,6-di-2-ithienyl-2,3-dihydropyrazine**  
El Hag R., Abdusalam M. M., Acilan C., KAYI H., ÖZALP YAMAN Ş.  
POLYHEDRON, vol.170, pp.25-33, 2019 (SCI-Expanded)
- X. **Effect of chalcogen atoms on the electronic band gaps of donor-acceptor-donor type semiconducting polymers: a systematic DFT investigation**  
Ozkilinc O., KAYI H.  
JOURNAL OF MOLECULAR MODELING, vol.25, no.6, 2019 (SCI-Expanded)
- XI. **Innovative Carbon Dioxide-Capturing Organic Solvent: Reaction Mechanism and Kinetics**  
YÜKSEL ORHAN Ö., Tankal H., KAYI H., Alper E.  
CHEMICAL ENGINEERING & TECHNOLOGY, vol.40, no.4, pp.737-744, 2017 (SCI-Expanded)
- XII. **Design of novel tellurium and selenium containing semiconducting polymers using quantum mechanical tools**  
Kaya B., KAYI H.  
COMPUTATIONAL AND THEORETICAL CHEMISTRY, vol.1099, pp.45-54, 2017 (SCI-Expanded)
- XIII. **Kinetics of CO<sub>2</sub> capture by carbon dioxide binding organic liquids: Experimental and molecular modelling studies**  
YÜKSEL ORHAN Ö., Tankal H., KAYI H., Alper E.  
INTERNATIONAL JOURNAL OF GREENHOUSE GAS CONTROL, vol.49, pp.379-386, 2016 (SCI-Expanded)
- XIV. **Kinetics of CO<sub>2</sub> Capture by Carbon Dioxide Binding Organic Liquids**  
YÜKSEL ORHAN Ö., KAYI H., Alper E.  
ENERGY, TRANSPORTATION AND GLOBAL WARMING, vol.PartF2, pp.591-603, 2016 (SCI-Expanded)
- XV. **Experimental and theoretical investigation of the reaction between CO<sub>2</sub> and carbon dioxide binding organic liquids**  
Tankal H., YÜKSEL ORHAN Ö., Alper E., ÖZDOĞAN T., KAYI H.  
TURKISH JOURNAL OF CHEMISTRY, vol.40, no.5, pp.706-719, 2016 (SCI-Expanded)
- XVI. **Correlations between hardness, electrostatic interactions, and thermodynamic parameters in the**

**decomposition reactions of 3-buten-1-ol, 3-methoxy-1-propene, and ethoxyethene**

Hasanzadeh N., Nori-Shargh D., KAYI H., Javid N. R.

STRUCTURAL CHEMISTRY, vol.26, no.2, pp.547-554, 2015 (SCI-Expanded)

- XVII. **Spectroelectrochemical Investigation of Nuclease Active Pt(II) Complexes Containing Pyrrole Oxime**  
Erdogan D. A., KAYI H., ÖZALP YAMAN Ş.  
ELECTROCHIMICA ACTA, vol.158, pp.333-341, 2015 (SCI-Expanded)
- XVIII. **A theoretical investigation of 4,7-di(furan-2-yl)benzo[c][1,2,5]selenadiazole-based donor-acceptor type conjugated polymer**  
KAYI H., Elkamel A.  
COMPUTATIONAL AND THEORETICAL CHEMISTRY, vol.1054, pp.38-45, 2015 (SCI-Expanded)
- XIX. **A computational study on 4,7-di(furan-2-yl)benzo[c][1,2,5]thiadiazole monomer and its oligomers**  
KAYI H.  
JOURNAL OF MOLECULAR MODELING, vol.20, no.6, 2014 (SCI-Expanded)
- XX. **Conformational behaviors of trans-2,3-and trans-2,5-dihalo-1,4-diselenanes. A complete basis set, hybrid-density functional theory study and natural bond orbital interpretations**  
Nori-Shargh D., Mousavi S. N., KAYI H.  
JOURNAL OF MOLECULAR MODELING, vol.20, no.5, 2014 (SCI-Expanded)
- XXI. **Deviations from Born-Oppenheimer Theory in Structural Chemistry: Jahn-Teller, Pseudo Jahn-Teller, and Hidden Pseudo Jahn-Teller Effects in C<sub>3</sub>H<sub>3</sub> and C<sub>3</sub>H<sub>3</sub>-**  
KAYI H., Garcia-Fernandez P., Bersuker I. B., Boggs J. E.  
JOURNAL OF PHYSICAL CHEMISTRY A, vol.117, no.36, pp.8671-8679, 2013 (SCI-Expanded)
- XXII. **Natural bond orbital, nuclear magnetic resonance analysis and hybrid-density functional theory study of sigma-aromaticity in Al<sub>2</sub>F<sub>6</sub>, Al<sub>2</sub>Cl<sub>6</sub>, Al<sub>2</sub>Br<sub>6</sub> and Al<sub>2</sub>I<sub>6</sub>**  
Nori-Shargh D., Yahyaei H., Mousavi S. N., Maasoomi A., KAYI H.  
JOURNAL OF MOLECULAR MODELING, vol.19, no.6, pp.2549-2557, 2013 (SCI-Expanded)
- XXIII. **Pseudo Jahn-Teller origin of bending instability of triatomic molecules**  
KAYI H., Bersuker I. B., Boggs J. E.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1023, pp.108-114, 2012 (SCI-Expanded)
- XXIV. **A theoretical investigation of the relative stability of hydrated glycine and methylcarbamic acid-from water clusters to interstellar ices**  
KAYI H., Kaiser R. I., Head J. D.  
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol.14, no.14, pp.4942-4958, 2012 (SCI-Expanded)
- XXV. **AM1\*parameters for palladium and silver**  
KAYI H., Clark T.  
JOURNAL OF MOLECULAR MODELING, vol.17, no.10, pp.2585-2600, 2011 (SCI-Expanded)
- XXVI. **A computational study on the structures of methylamine-carbon dioxide-water clusters: evidence for the barrier free formation of the methylcarbamic acid zwitterion (CH<sub>3</sub>NH<sub>2</sub>+COO<sup>-</sup>) in interstellar water ices**  
KAYI H., Kaiser R. I., Head J. D.  
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol.13, no.23, pp.11083-11098, 2011 (SCI-Expanded)
- XXVII. **A theoretical investigation of the low energy conformers of the isomers glycine and methylcarbamic acid and their role in the interstellar medium**  
KAYI H., Kaiser R. I., Head J. D.  
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol.13, no.35, pp.15774-15784, 2011 (SCI-Expanded)
- XXVIII. **AM1\*parameters for manganese and iron**  
KAYI H., Clark T.  
JOURNAL OF MOLECULAR MODELING, vol.16, no.6, pp.1109-1126, 2010 (SCI-Expanded)
- XXIX. **AM1\*parameters for gold**  
KAYI H.  
JOURNAL OF MOLECULAR MODELING, vol.16, no.5, pp.1029-1038, 2010 (SCI-Expanded)
- XXX. **AM1\*parameters for cobalt and nickel**

- KAYI H., Clark T.  
JOURNAL OF MOLECULAR MODELING, vol.16, no.1, pp.29-47, 2010 (SCI-Expanded)
- XXXI. **AM1\*parameters for vanadium and chromium**  
KAYI H., Clark T.  
JOURNAL OF MOLECULAR MODELING, vol.15, no.10, pp.1253-1269, 2009 (SCI-Expanded)
- XXXII. **AM1\*parameters for bromine and iodine**  
KAYI H., Clark T.  
JOURNAL OF MOLECULAR MODELING, vol.15, no.3, pp.295-308, 2009 (SCI-Expanded)
- XXXIII. **Ni(II), Cu(II), and Zn(II) Complexes of Tetradentate Schiff Base Containing Two Thiadiazoles Units: Structural, Spectroscopic, Magnetic Properties, and Molecular Modeling Studies**  
SERBEST K., KAYI H., Er M., SANCAK K., DEĞİRMENCİOĞLU İ.  
HETEROATOM CHEMISTRY, vol.19, no.7, pp.700-712, 2008 (SCI-Expanded)
- XXXIV. **AM1\*parameters for copper and zinc**  
KAYI H., Clark T.  
JOURNAL OF MOLECULAR MODELING, vol.13, no.9, pp.965-979, 2007 (SCI-Expanded)
- XXXV. **Prediction of lower critical solution temperature of N-isopropylacrylamide-acrylic acid copolymer by an artificial neural network model**  
KAYI H., Tuncel S., Elkamel A., Alper E.  
JOURNAL OF MOLECULAR MODELING, vol.11, no.1, pp.55-60, 2005 (SCI-Expanded)
- XXXVI. **Stimuli-responsive properties of aminophenylboronic acid-carrying thermosensitive copolymers**  
Uguzdogan E., KAYI H., Denkbaz E., Patir S., Tuncel A.  
POLYMER INTERNATIONAL, vol.52, no.5, pp.649-657, 2003 (SCI-Expanded)

## Articles Published in Other Journals

- I. **Theoretical investigation of carbon dioxide capture by aqueous boric acid solution: A termolecular reaction mechanism**  
KAYI H.  
BOR DERGİSİ, vol.3, no.1, pp.1-7, 2018 (Peer-Reviewed Journal)
- II. **Design and Simulation of Semiconducting Polymers for Optoelectronic Applications by Using Quantum Mechanical Tools**  
Özkılınç Ö., Kaya B., KAYI H.  
Journal of Turkish Chemical Society, Section:B Chemical Engineering, vol.1, no.1, pp.127-134, 2017 (Peer-Reviewed Journal)

## Books

- I. **Kinetics of CO<sub>2</sub> capture by carbon dioxide binding organic liquids**  
YÜKSEL ORHAN Ö., KAYI H., ALPER E.  
in: Energy, Transportation and Global Warming, Green Energy and Technology, Panagiotis Grammelis, Editor, Springer International Publishing, pp.591-603, 2016
- II. **Fluorimetry**  
KAYI H.  
in: Instrumental Analysis Laboratory, Ayhan Hakan, Koçum Cengiz, Editor, Aydan Basımevi, Ankara, Ankara, pp.29-36, 2004

## Papers Published in Refereed Scientific Meetings

- I. **Prediction of Chemical Oxygen Demand from the Chemical Composition of Wastewater by Artificial Neural Networks**  
Saleh B. A., KAYI H.  
1st Iraqi Academics Syndicate International Conference for Pure and Applied Sciences, IICPS 2020, Babylon, Virtual, Iraq, 5 - 06 December 2020, vol.1818
- II. **Artificial Neural Network Prediction of Sulfur Content of Diesel fuel from its Physical Properties**  
Younis Y. M., KAYI H.  
2nd International Conference on Sustainable Engineering Techniques (ICSET), Baghdad, Iraq, 6 - 07 March 2019, vol.518
- III. **Quantum chemical investigation of amino acid detection and formation in low temperature molecular ices typically present in the Outer Solar System**  
Head J. D., KAYI H., Kaiser R. I.  
245th National Spring Meeting of the American-Chemical-Society (ACS), Louisiana, United States Of America, 7 - 11 April 2013, vol.245

## Supported Projects

Kayi H., Özalp Yaman Ş., TUBITAK Project, Synthesis of new molecules with quorum sensing inhibitory properties and their use in development of an eco-friendly hydrogel paint system (TÜBİTAK1001 Project No:123Z892), 2024 - 2026

Kayi H., Özalp Yaman Ş., TUBITAK Project, Kurşun içermeyen yeni nesil primer patlayıcı tasarımı, sentezi ve karakterizasyonu (TÜBİTAK1001 Proje No: 117Z391), 2017 - 2022

Kayi H., TUBITAK Project, Yeni yarıiletken konjüge polimerlerin tasarımı ve elektronik ve optik özelliklerinin kuantum kimyasal yöntemlerle sistematik olarak incelenmesi (TÜBİTAK3501 Proje No: 117Z354), 2017 - 2021

Kayi H., Alper E., TUBITAK Project, Karbon dioksit yakalayan organik sıvıların reaksiyon kinetiği ve mekanizmasının deneysel ve moleküler modelleme yöntemleriyle incelenmesi (TÜBİTAK1001 Proje No: 213M390), 2014 - 2016

Kayi H., Clark T., Other International Funding Programs, Parameterization of AM1 for Redox-Active Metals (Almanya, Deutsche Forschungsgemeinschaft DFG, GK312-Homogeneous and Heterogeneous Electron Transfer, SFB583-Redox-Active Metal Complexes), 2004 - 2009

Kayi H., Alper E., TUBITAK Project, N-izopropil akril amid akrilik asit kopolimerinin alt kritik çözelti sıcaklığının yapay sinir ağları ile tahmini (TÜBİTAK Proje No: MİSAG 242, 102M088), 2003 - 2004

## Peer Reviews in Scientific Publications

JOURNAL OF MATERIALS CHEMISTRY A, Journal Indexed in SCI-E, November 2022

RSC ADVANCES, Journal Indexed in SCI-E, March 2022

JOURNAL OF MOLECULAR MODELING, Journal Indexed in SCI-E, September 2021

CHEMICAL COMMUNICATIONS, Journal Indexed in SCI-E, August 2021

JOURNAL OF MOLECULAR STRUCTURE, Journal Indexed in SCI-E, January 2021

TURKISH JOURNAL OF CHEMISTRY, Journal Indexed in SCI-E, October 2019

Physical Chemistry Research, Journal Indexed in ESCI, April 2018

JOURNAL OF APPLIED POLYMER SCIENCE, Journal Indexed in SCI-E, April 2018

NEW JOURNAL OF CHEMISTRY, Journal Indexed in SCI-E, May 2017

SPECTROCHIMICA ACTA - PART A: MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, Journal Indexed in SCI-E, January 2016

CANADIAN JOURNAL OF CHEMISTRY, Journal Indexed in SCI-E, August 2015

JOURNAL OF PHYSICAL CHEMISTRY, Journal Indexed in SCI-E, March 2014

ENVIRONMENTAL ENGINEERING AND MANAGEMENT JOURNAL, Journal Indexed in SCI-E, January 2014

## Metrics

Publication: 43

Citation (WoS): 363

Citation (Scopus): 379

H-Index (WoS): 13

H-Index (Scopus): 12

## Congress and Symposium Activities

IX. National Inorganic Chemistry Congress, Attendee, Ankara, Turkey, 2024

2nd International Natural Science, Engineering and Material Technologies Conference, NEM2022, Attendee, Kırklareli, Turkey, 2022

14. Ulusal Kimya Mühendisliği Kongresi, UKMK2020, Attendee, Konya, Turkey, 2021

14. Ulusal Kimya Mühendisliği Kongresi, UKMK2020, Attendee, Konya, Turkey, 2021

XV. International Conference on Chemical and Environmental Engineering, ICCEE2021, Attendee, Dubai, United Arab Emirates, 2021

Iraqi Academics Syndicate International Conference for Pure and Applied Sciences (IICPS), Attendee, Al Hillah, Iraq, 2020

34th Molecular Modeling Workshop, MMWS2020, Attendee, Erlangen, Germany, 2020

34th Molecular Modeling Workshop, MMWS2020, Attendee, Erlangen, Germany, 2020

Advanced Electronic Structure Methods in Condensed Matter Physics, ESCOMP-2019, Attendee, Lausanne, Switzerland, 2019

33rd Molecular Modeling Workshop and Symposium in Honor of Tim Clark's 70th Birthday, MMWS2019, Attendee, Erlangen, Germany, 2019

7th Drug Chemistry Conference: Design, Synthesis, Production and Standardization of Drug Active Substances, Attendee, Antalya, Turkey, 2019

2nd International Conference on Sustainable Engineering Techniques, ICSET-2019, Attendee, Baghdad, Iraq, 2019

International Computational Science Congress, CSC-2018, Attendee, Amasya, Turkey, 2018

International Computational Science Congress, CSC-2018, Attendee, Amasya, Turkey, 2018

12th Chemical Physics Congress, CPC-XII, Attendee, Karabük, Turkey, 2018

5th International Conference on Computation for Science and Technology, Attendee, Antalya, Turkey, 2018

13. Ulusal Kimya Mühendisliği Kongresi, UKMK2018, Attendee, Van, Turkey, 2018

5th BAU Drug Design Congress, Working Group, İstanbul, Turkey, 2017

3. Hesaplamalı Kimya Kongresi, Attendee, Ankara, Turkey, 2017

3. Hesaplamalı Kimya Kongresi, Attendee, Ankara, Turkey, 2017

3. Hesaplamalı Kimya Kongresi, Attendee, Ankara, Turkey, 2017

12. Ulusal Kimya Mühendisliği Kongresi, Attendee, İzmir, Turkey, 2016

6. Ulusal Hava Kirliliği ve Kontrolü Sempozyumu, Attendee, İzmir, Turkey, 2015

2. Ulusal Hesaplamalı Kimya Kongresi, Attendee, Kars, Turkey, 2015

Global Conference on Global Warming, GCGW2015, Working Group, Athens, Greece, 2015

5. Fiziksel Kimya Kongresi, Attendee, Konya, Turkey, 2015

Molecular Electronic Structure Workshop MES2014, Attendee, Amasya, Turkey, 2014

25th Austin Symposium on Molecular Structure and Dynamics at Dallas, Attendee, Texas, United States Of America, 2014

American Chemical Society, 245th ACS Meeting, Attendee, Louisiana, United States Of America, 2013

XXIth International Symposium on the Jahn-Teller Effect, Attendee, Tsukuba, Japan, 2012

American Chemical Society, SWRM2011 67th ACS Southwest Meeting, Attendee, Texas, United States Of America, 2011

Pacificchem 2010, Attendee, Hawaii, United States Of America, 2010

Modeling'09 Conference, Attendee, Erlangen, Germany, 2009

UKMK-8, Ulusal Kimya Mühendisliği Kongresi, Attendee, Malatya, Turkey, 2009



22th Darmstadter Molecular Modeling Workshop, Attendee, Erlangen, Germany, 2008  
21th Darmstadter Molecular Modeling Workshop, Attendee, Erlangen, Germany, 2007  
20th Darmstadter Molecular Modeling Workshop, Attendee, Erlangen, Germany, 2006  
UKMK-5, Ulusal Kimya Mühendisliği Kongresi, Attendee, Ankara, Turkey, 2002

## **Scholarships**

Postdoctoral Research Fellowship, Official Institutions of Foreign Countries, 2010 - 2011  
Ph.D. Scholarship, Official Institutions of Foreign Countries, 2004 - 2009