

Assoc. 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 1998 - 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

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

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

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

Kimyasal Hesaplamalar, Doctorate, 2013 - 2014

Advising Theses

Kayı H., Not defined., Doctorate, E.NUR(Student), Continues

Kayı H., Metal Organic Framework Based Fertilizer Production: Molecular Simulation and Controlled Release Applications, Doctorate, R.TAŞ(Student), Continues

KAYI H., Benzokalkojendiazol bazlı 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 artifical 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. Ti-substituted organosilica membranes for H₂ sieving: Sol-gel and DFT insights

Kayı H., Kaya P., Kurt T., Mirza E.Ş., Topuz B.

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

II. 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)

III. Design of a Zr-based metal-organic framework as an efficient fosfomycin carrier: a combined

experimental and DFT study

Topuz B., Kayı H., Şahin T., Ersoy F. Ş., Günyaktı A., Karakeçili A.

NEW JOURNAL OF CHEMISTRY, vol.47, no.3, pp.1278-1290, 2023 (SCI-Expanded)

IV. 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)

V. 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)

VI. Capture of Carbonyl Sulfide by Organic Liquid Mixtures: A Systematic DFT Investigation

Abduessim M., KAYI H.

INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH, vol.60, no.3, pp.1366-1374, 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. Radicalic 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)

IX. 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)

X. 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)

XI. 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)

XII. Kinetics of CO₂ 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)

XIII. Kinetics of CO₂ 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)

XIV. Experimental and theoretical investigation of the reaction between CO₂ 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)

XV. 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)

XVI. 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)

XVII. 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)
- XVIII. **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)
- XIX. **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)
- XX. **Deviations from Born-Oppenheimer Theory in Structural Chemistry: Jahn-Teller, Pseudo Jahn-Teller, and Hidden Pseudo Jahn-Teller Effects in C₃H₃ and C₃H₃-**
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)
- XXI. **Natural bond orbital, nuclear magnetic resonance analysis and hybrid-density functional theory study of sigma-aromaticity in Al₂F₆, Al₂Cl₆, Al₂Br₆ and Al₂I₆**
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)
- XXII. **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)
- XXIII. **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)
- XXIV. **AM1*parameters for palladium and silver**
KAYI H., Clark T.
JOURNAL OF MOLECULAR MODELING, vol.17, no.10, pp.2585-2600, 2011 (SCI-Expanded)
- XXV. **A computational study on the structures of methylamine-carbon dioxide-water clusters: evidence for the barrier free formation of the methylcarbamic acid zwitterion (CH₃NH₂⁺COO⁻) 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)
- XXVI. **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)
- XXVII. **AM1*parameters for manganese and iron**
KAYI H., Clark T.
JOURNAL OF MOLECULAR MODELING, vol.16, no.6, pp.1109-1126, 2010 (SCI-Expanded)
- XXVIII. **AM1*parameters for gold**
KAYI H.
JOURNAL OF MOLECULAR MODELING, vol.16, no.5, pp.1029-1038, 2010 (SCI-Expanded)
- XXIX. **AM1*parameters for cobalt and nickel**
KAYI H., Clark T.
JOURNAL OF MOLECULAR MODELING, vol.16, no.1, pp.29-47, 2010 (SCI-Expanded)
- XXX. **AM1*parameters for vanadium and chromium**
KAYI H., Clark T.
JOURNAL OF MOLECULAR MODELING, vol.15, no.10, pp.1253-1269, 2009 (SCI-Expanded)
- XXXI. **AM1*parameters for bromine and iodine**
KAYI H., Clark T.

- JOURNAL OF MOLECULAR MODELING, vol.15, no.3, pp.295-308, 2009 (SCI-Expanded)
- XXXII. **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., DEĞİRMENÇİOĞLU İ.
HETEROATOM CHEMISTRY, vol.19, no.7, pp.700-712, 2008 (SCI-Expanded)
- XXXIII. **AM1*parameters for copper and zinc**
KAYI H., Clark T.
JOURNAL OF MOLECULAR MODELING, vol.13, no.9, pp.965-979, 2007 (SCI-Expanded)
- XXXIV. **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)
- XXXV. **Stimuli-responsive properties of aminophenylboronic acid-carrying thermosensitive copolymers**
Uguzdogan E., KAYI H., Denkbas 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**
Özkilinç 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 & Book Chapters

- I. **Kinetics of CO₂ 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

Refereed Congress / Symposium Publications in Proceedings

- 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 tasarımlı, sentezi ve
karakterizasyonu (TÜBİTAK1001 Proje No: 117Z391), 2017 - 2022

Kayi H., TUBITAK Project, Yeni yarıiletken konjuge polimerlerin tasarımları 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

Scientific Refereeing

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: 42

Citation (WoS): 351

Citation (Scopus): 262

H-Index (WoS): 13

H-Index (Scopus): 11

Congress and Symposium Activities

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

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

Model(l)ing'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