Assoc. Prof. Dr. Hakan KAYI

Ankara University, Chemical Engineering Department, Ankara, Turkey

EDUCATION

Ph.D.	Computer-Chemie-Centrum	Friedrich-Alexander Universität Erlangen-Nürnberg, Germany	2009
M.Sc.	Chemical Engineering Department	Hacettepe University	2003
B.Sc.	Chemical Engineering Department	Hacettepe University	2000

EMPLOYMENT

Assoc. Prof. Dr.	Chemical Engineering Department	Ankara University	2018-…
Asst. Prof. Dr.	Chemical Engineering Department	Ankara University	2018-2018
Asst. Prof. Dr.	Chemical Engineering and Applied Chemistry Department	Atılım University	2013-2018
Postdoctoral Research Associate	Institute for Theoretical Chemistry	University of Texas at Austin, USA	2011-2013
Postdoctoral Research Fellow	W.M. Keck Research Laboratory in Astrochemistry	University of Hawaii at Manoa, USA	2010-2011
Research Assistant	Computer-Chemie-Centrum	Friedrich-Alexander Universität Erlangen-Nürnberg, Germany	2004-2009
Research Assistant	Chemical Engineering Department	Hacettepe University	2001-2004

RESEARCH INTERESTS

Computational materials science and engineering.
Molecular design, molecular modeling, reaction simulation.
Design, modeling and simulation of semiconducting polymers for solar cells and electrochromic device applications.
Carbon dioxide and carbonyl sulfide capture, storage, reaction mechanisms and kinetics of carbon dioxide binding organic liquids.
Astrochemical reactions.
Vibronic interactions and pseudo Jahn-Teller effect.
Anti-cancer drug design and simulation of drug-DNA interactions.
Artificial neural networks applications in chemical engineering.
Quantum mechanical method development.

PROJECTS

Project Title	Supporting Organization	Role	Date
Design of novel semiconducting conjugated polymers and systematical investigation of their electronic and optical properties by quantum chemical methods (Project No: 117Z354)	TÜBİTAK (3501)	Principal Investigator	2017-…
Design, synthesis and characterization of new generation explosives without lead (Project No: 117Z391)	TÜBİTAK (1001)	Researcher	2017-…
Experimental and molecular modeling studies of reaction kinetics and mechanism of carbon dioxide binding organic liquids (Project No: 213M390)	TÜBİTAK (1001)	Researcher	2014-2016
Parameterization of AM1* for redox-active metals (Project No: CI85171)	Deutsche Forschungsgemeinschaft (DFG), Germany	Researcher	2006-2009
Prediction of lower critical solution temperature of N-izopropylacrylamid-acrylic acid polymer by artificial neural networks (Project No: MISAG242)	TÜBİTAK (MISAG)	Researcher	2002-2003

THESES SUPERVISED

1. Rabia Elhag (Ph.D.), *Design of novel platinum and palladium complexes containing pyridyl type ligands for cancer tumor treatment using molecular modeling approach*, 2015-2018.

2. Mahmoud Abduesslam (Ph.D.), *Theoretical investigation of carbonyl sulfide capture by organic solvents*, 2017-cont.

3. Basim Ahmed Saleh Alobaidi (M.Sc.), *Prediction of chemical oxygen demand from the chemical composition of waste water by artificial neural networks*, 2017-2019.

4. Hawa Ahmed (M.Sc.), *Prediction of kinematic viscosity of petroleum fractions*, 2016-2018.

5. Younis Muhsin Younis Al-Ani (M.Sc.), *Neural network prediction of flash point of diesel fuel from its composition*, 2016-2017.

6. Abubaker Bushra Ali Mehasi (M.Sc.), *Recovery of silver from silver oxide batteries: A combined theoretical and experimental study,* 2015-2017.

7. Ali Gerra Almuamri (M.Sc.), *Modeling and simulation of a vacuum distillation unit in an oil refinery,* 2015-2017.

8. Khaled Sowani (M.Sc.), *Design and optmization of an atmospheric distillation unit in an oil refinery*, 2015-2017.

9. Abubaker Hadia (M.Sc.), *Theoretical investigation of carbonyl sulfide capture by aqueous diethanolamine solution*, 2015-2017.

10. Hilal Tankal (M.Sc.), *Quantum mechanical investigation of reaction mechanisms of carbon dioxide binding organic liquids,* 2014-2016 (2nd advisor)

PUBLICATIONS

SCI & SCI-Exp

1) Ö. Özkılınç, **H. Kayı (2019)** Effect of chalcogen atoms on the electronic band gap of the donor-acceptor-donor type semiconducting polymers: A systematic DFT investigation, *Journal of Molecular Modeling*, 25:167. DOI:10.1007/s00894-019-4043-2

2) R. Elhag, M.M. Abdusalam, C. Acilan, **H. Kayı**, Ş. Özalp-Yaman **(2019)** Radicalic cleavage pathway and DNA docking studies of novel chemotherapic platinum agent of 5,6-2-di-2-ithienyl-2,3-dihydropyrazine, *Polyhedron*, 170:25-33. DOI:10.1016/j.poly.2019.04.054

3) Ö. Y.-Orhan, H. Tankal, **H. Kayı**, E. Alper **(2017)** Innovative Carbon Dioxide-Capturing Organic Solvent: Reaction Mechanism and Kinetics, *Chemical Engineering & Technology*, 40(4): 737-744.

4) B. Kaya, **H. Kayı (2017)** Design of novel tellurium and selenium containing semiconducting polymers using quantum mechanical tools, *Computational and Theoretical Chemistry*, 1099: 45-54.

5) H. Tankal, Ö. Y.-Orhan, E. Alper, T. Özdoğan, **H. Kayı (2016)** Experimental and theoretical investigation of reaction between CO2 and carbon dioxide binding organic liquids, *Turkish Journal of Chemistry*, 40(5): 706-719

6) Ö. Y.-Orhan, H. Tankal, **H. Kayı**, E. Alper **(2016)** Kinetics of CO2 capture by carbon dioxide binding organic liquids: Experimental and molecular modeling studies, *International Journal of Greenhouse Gas Control*, 49: 379–386

7) D. Erdoğan Altunöz, **H. Kayı**, Ş. Özalp-Yaman **(2015)** Spectroelectrochemical investigation of nuclease active Pt(II) complexes containing pyrrole oxime. *Electrochimica Acta*, 158: 333-341.

8) H. Kayı, A. Elkamel **(2015)** A theoretical investigation of 4,7-di(furan-2-yl)benzo[c] [1,2,5] selenadiazole-based donor-acceptor type conjugated polymer. *Computational and Theoretical Chemistry*, 1054: 38-45.

9) N. Hasanzadeh, D. Nori-Shargh, **H. Kayı,** N. Rezaeijavid **(2015)** Correlations between hardness, electrostatic interactions and thermodynamic parameters in the decomposition reactions of 3-buten-1-ol, 3-methoxy-1-propene and ethoxyethene. *Structural Chemistry,* 26(2): 547-554.

10) H. Kayı (2014) A computational study on 4,7-di(furan-2-yl) benzo[c] [1,2,5]thiadiazole monomer and its oligomers. *Journal of Molecular Modeling*, 20(6): 2269.

11) D. Nori-Shargh, S.N. Mousavi, **H. Kayı (2014)** 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. *Journal of Molecular Modelling,* 20(5): 2249.

12) H. Kayı; P. Garcia-Fernandez, I.B. Bersuker, J.E. Boggs **(2013)** Deviations from Born-Oppenheimer theory: Jahn-Teller, pseudo Jahn-Teller and hidden pseudo Jahn-Teller effects in C_3H_3 and $C_3H_3^-$. *Journal of Physical Chemistry A,* 117(36): 8671-8679.

13) D. Nori-Shargh, H.Yahyaei, S. N. Mousavi, A. Maasoomi, **H. Kayı (2013)** Natural bond orbital, nuclear magnetic resonance analysis and hybrid-density functional theory study of σ-aromaticity in Al_2F_6, Al_2Cl_6, Al_2Br_6 and Al_2I_6 dimers. *Journal of Molecular Modeling,* 19(6):2549-2557.

14) H. Kayı, I.B. Bersuker, J.E. Boggs **(2012)** Pseudo Jahn-Teller explanation of bending instability of triatomic molecules. *Journal of Molecular Structure,* 1023:108-114.

15) H. Kayı, R.I. Kaiser, J.D. Head **(2012)** A theoretical investigation of the relative stability of hydrated glycine and methylcarbamic acid: from water clusters to interstellar ices. *Physical Chemistry Chemical Physics,* 14(14):4942-4958.

16) H. Kayı, R.I. Kaiser, J.D. Head **(2011)** A theoretical investigation of the low energy conformers of the isomers glycine and methylcarbamic acid and their role in the interstellar medium. *Physical Chemistry Chemical Physics,* 13(35): 15774-15784.

17) H. Kayı, R.I. Kaiser, J.D. Head **(2011)** A computational study on the structures of methylamine–carbon dioxide–water clusters: evidence for the barrier free formation of the methylcarbamic acid zwitterion ($CH_3NH_2^+COO^-$) in interstellar water ices. *Physical Chemistry Chemical Physics,* 13(23):11083-11098.

18) H. Kayı, T. Clark **(2011)** AM1* parameters for palladium and silver. *Journal of Molecular Modeling,* 17(10):2585-2600.

18) H. Kayı, T. Clark **(2010)** AM1* parameters for manganese and iron. *Journal of Molecular Modeling,* 16(6):1109-1126.

20) H. Kayı (2010) AM1* parameters for gold. *Journal of Molecular Modeling,* 16(5):1029-1038.

21) H. Kayı, T. Clark **(2010)** AM1* parameters for cobalt and nickel. *Journal of Molecular Modeling,* 16(1):29-47.

22) H. Kayı, T. Clark **(2009)** AM1* parameters for vanadium and chromium. *Journal of Molecular Modeling,* 15(10):1253-1269.

23) H. Kayı, T. Clark **(2009)** AM1* parameters for bromine and iodine. *Journal of Molecular Modeling,* 15(3):295-308.

24) K. Serbest, **H. Kayı**, M. Er, K. Sancak, I. Değirmencioğlu **(2008)** Ni(II), Cu(II) and Zn(II) complexes of tetradentate schiff base containing two thiadiazoles units: structural, spectroscopic, magnetic properties and molecular modeling studies. *Heteroatom Chemistry,* 19(7):700-712.

25) H. Kayı, T. Clark **(2007)** AM1* parameters for copper and zinc. *Journal of Molecular Modeling,* 13(9):965-979.

26) H. Kayı, A. Elkamel, S.A. Tuncel, E. Alper **(2005)** Prediction of lower critical solution temperature of N-isopropylacrylamide-acrylic acid copolymer by an artificial neural network model *Journal of Molecular Modeling,* 11(1):55-60.

27) E. Uğuzdoğan, **H. Kayı**, E.B. Denkbaş, S. Patır, A. Tuncel **(2003)** Stimuli-responsive properties of aminophenylboronic acid-carrying thermosensitive copolymers. *Polymer International,* 52(5):649-657.

International Refereed Journal Articles

1) Younis Muhsin Younis Al-ani, **H. Kayı (2019)** Artificial neural network prediction of sulfur content of diesel fuel from its physical properties, IOP Conf. Series: *Materials Science and Engineering*, 518:062008. DOI:10.1088/1757-899X/518/6/062008

National Refereed Journal Articles

1) H. Kayı (2018) Theoretical investigation of carbon dioxide capture by aqueous boric acid solution: A termolecular reaction mechanism, Journal of Boron, 03(01), pp. 1-7

2) Ö. Özkılınç, B. Kaya, **H. Kayı (2017)** Design and simulation of semiconducting polymers for optoelectronic applications by using quantum mechanical tools, *Journal of the Turkish Chemical Society, Section:B Chemical Engineering*, 1(1):127-134

Book Chapter (International)

Ö. Y-Orhan, **H. Kayı**, E. Alper (Editör: Grammelis, Panagiotis) **(2016)** "Kinetics of CO2 capture by carbon dioxide binding organic liquids", in *Energy, Transportation and Global Warming, Green Energy and Technology*, pp. 591-603, ISBN:978-3-319-30126-6, Springer International Publishing, Switzerland, DOI:10.1007/978-3-319-30127-3_43

Book Chapter (National)

H. Kayı (2004) "Fluorimetry", in *Instrumental Analysis Laboratory*, (Editörler: Hakan Ayhan & Cengiz. Koçum) pp. 29-37; ISBN:975-98530-0-0, Aydan Publishings, Ankara.

Presentations (International Conferences)

1) Ö. Özkılınç, **H. Kayı (2019)** Advanced Electronic Structure Methods in Condensed Matter Physics, ESCOMP-2019, **Lausanne, Switzerland**, July 08-10, "A DFT investigation of the electronic band gap of 4,7-bis(2,3-dihydrothieno[3,4-b]-1,4-dioxin-5-yl)benzo[2,1,5]-oxadiazole", page 25, Poster Presentation.

2) H. Kayı, Ö. Özkılınç **(2019)** 33rd Molecular Modeling Workshop and Symposium in Honor of Tim Clark's 70th Birthday, 33rdMMWS2019, **Erlangen, Germany**, April 08-11, "Design of the tellurium-containing semiconducting polymers", page 45, Oral Presentation.

3) Younis Muhsin Younis Al-ani, **H. Kayı (2019)** 2nd International Conference on Sustainable Engineering Techniques, ICSET-2019, **Baghdad, Iraq**, March 06-07, "Artificial neural network prediction of sulfur content of diesel fuel from its physical properties", Oral Presentation ID: 198.

4) Ö. Özkılınç, **H. Kayı (2018)** International Computational Science Congress, CSC-2018, **Amasya**,**Türkiye**, October 26-28, "Theoretical investigation of electronic properties of the 4,7-bis(2,3-dihydro-seleno[3,4-b]-1,4-dioxin-5-yl) benzo[2,1,5]-selenadiazole conjugated polymer", Oral Presentation.
5) Ö. Özkılınç, **H. Kayı (2018)** 12th Chemical Physics Congress, CPC-XII, **Safranbolu, Türkiye**, October 12-13, "Theoretical investigation of electronic properties of the ethylenedioxyselenophene containing donor-acceptor-donor type conjugated polymer", PP-32, page 83. Poster Presentation.

6) Ö. Özkılınç, **H. Kayı (2018)** 5th International Conference on Computation for Science and Technology, ICCST2018, Antalya, Türkiye, September 23-26, "Design of the donor-acceptor-donor type semiconducting polymer 4,7-di(furan-2-yl)benzo[c]telluradiazole by density functional theory", Oral Presentation No: OP-13, page 46.

7) Ö. Y-Orhan, **H. Kayı**, E. Alper **(2015)** Global Conference on Global Warming, GCGW2015, **Athens, Greece**, May 24-27. "*Kinetics of CO2 capture by carbon dioxide binding organic liquids*", Sub. No:61.

8) H. Kayı (2014) Molecular Electronic Structure Workshop MES2014, **Amasya**, **Türkiye**, September 01-05. "*Calculation of the band gap of 4,7-di(furan-2-yl)benzo[co][1,2,5]thiadiazole polymer: a DFT approach*", Page 52.

9) H. Kayı, J. E. Boggs, I.B. Bersuker **(2014)** 25th Austin Symposium on Molecular Structure and Dynamics at Dallas, **Texas, USA**, March 1-3., "*Origin of Bending Instability of Small Linear Molecules and Deviations from Born-Oppenheimer Theory: pseudo Jahn-Teller Effect*", Lecture:10, Page 35.

10) J.D. Head, **H. Kayı**, R.I. Kaiser **(2013)** American Chemical Society, 245th ACS Meeting, New Orleans, LA, USA, April 7-13. "*Quantum chemical investigation of amino acid detection and formation in low temperature molecular ices typically present in the Outer Solar System*" Session: Physical Chemistry, Presentation No: PHYS-292.

11) H. Kayı, J. E. Boggs, I.B. Bersuker **(2012)** XXIth International Symposium on the Jahn-Teller Effect, **Tsukuba**, **Japan**, August 26-31, 2012. "*The origin of bending instability of triatomic molecules: pseudo Jahn-Teller effect*", Presentation No: P23.

12) H. Kayı, R.I. Kaiser, J.D. Head **(2011)** American Chemical Society, SWRM2011 67th ACS Southwest Meeting, Austin, Texas, USA, November 9-12, 2011. "*Theoretical investigation of the formation of the simple amino acids in extraterrestrial ices*" Session: Physical Chemistry, Presentation No: SWRM-571.

13) H. Kayı, R.I. Kaiser, J.D. Head **(2010)** Pacifichem 2010, Honolulu, **Hawaii**, **USA**, December 15-20. "*Theoretical investigation of the formation of the simple amino acid glycine and its isomers in extraterrestrial ices*", Session: Kuiper Belt Objects-Laboratory Studies, Models, Theory, and Observations, Presentation No:1353.

14) H. Kayı, T. Clark **(2009)** Model(l)ing'09 Conference, **Erlangen**, **Germany**, September 6-11. "*Parameterization of AM1**".

15) H. Kayı, T. Clark **(2008)** 22th Darmstadter Molecular Modeling Workshop, **Erlangen**, **Germany**, April 29-30. "*Parameterization of Bromine and Iodine for AM1**".

16) H. Kayı, T. Clark **(2007)** 21th Darmstadter Molecular Modeling Workshop, **Erlangen**, **Germany**, May 15-16. "*Parameterization of Zinc for AM1**".

17) H. Kayı, T. Clark **(2006)** 20th Darmstadter Molecular Modeling Workshop, **Erlangen**, **Germany**, May 23-24. "*Parameterization of Copper for AM1**".

Presentations (National Conferences)

1) Ö. Özkılınç, **H. Kayı (2018)** 13. Ulusal Kimya Mühendisliği Kongresi, UKMK2018, 03-06 Eylül 2018, Van, P87, sayfa 5830, "Bazı yeni oksadiazol içeren yarıiletken polimerlerin DFT ile tasarımı ve simülasyonu"

2-a) A. Hadia, **H. Kayı (2017)** 3. Hesaplamalı Kimya Kongresi, 12-14 Ekim 2017, Ankara, sayfa 9, "*Dietanol amin çözeltisi ile karbonil sülfitin yakalanması*".

b) Ö. Özkılınç, **H. Kayı (2017)** 3. Hesaplamalı Kimya Kongresi, 12-14 Ekim 2017, Ankara, sayfa 42, "*Yoğunluk fonsiyoneli teorisi yardımıyla bazı yarıiletken polimerlerin tasarımı ve elektronik bant aralıklarının hesaplanması*".

c) B. Kaya, **H. Kayı (2017)** 3. Hesaplamalı Kimya Kongresi, 12-14 Ekim 2017, Ankara, sayfa 42, "*Selenofen selenadiazol ve tellurofen telluradiazol içeren yarıiletken polimerlerin yoğunluk fonsiyoneli teorisi ile tasarım ve benzetimi*".

3) B. Kaya, Ö. Özkılınç, **H. Kayı (2016)** 12. Ulusal Kimya Mühendisliği Kongresi, 23-26 Ağustos, İzmir, sayfa 648-653, "*Optoelektronik uygulamalar için yeni yarıiletken polimerlerin kuantum mekanik yöntemlerle tasarım ve simülasyonu*".

4) H. Tankal, Ö. Y-Orhan, E. Alper, **H. Kayı (2015)** 6. Ulusal Hava Kirliliği ve Kontrolü Sempozyumu, HKK 2015, 07-09 Ekim, İzmir, sayfa 750-754, "*TMBG Organik Çözücüsünün 1-Hekzanol ve 1-Propanol İçerisindeki CO_2 Tutma Mekanizmasının DFT Yöntemiyle İncelenmesi".*

5) H. Tankal, Ö. Y-Orhan, E. Alper, **H. Kayı (2015)** 2. Ulusal Hesaplamalı Kimya Kongresi, 02-05 Haziran, Kars, Sunum04, sayfa 10, *"DBN ile TBD organik çözücülerinin 1-Butanol ve 1-Propanol içerisindeki CO_2 tutma eğilimlerinin DFT yöntemleriyle incelenmesi"*.

6) H. Tankal, Ö. Y-Orhan, E. Alper, T. Özdoğan, **H. Kayı (2015)** 5. Fiziksel Kimya Kongresi, 16-19 Mayıs, Konya, Sunum30, sayfa 40, *"İki organik çözücünün CO_2 tutma eğilimlerinin kuantum mekanik yöntemlerle incelenmesi"*.

7) O. Bavbek, **H. Kayı**, E. Alper **(2008)** UKMK-8, Ulusal Kimya Mühendisliği Kongresi, Malatya, Türkiye, 26-29 Ağustos. "*İlaç endüstrisinde kullanılan akışkan yataklı kurutucunun yapay sinir ağları ile modellenmesi ve kurutma süresinin tahmini*", ARG-12.

8) H. Kayı, E. Elkamel, E. Alper **(2002)** UKMK-5, Ulusal Kimya Mühendisliği Kongresi, Ankara, Türkiye, 2-5 Eylül. "*N-izopropilakrilamid-akrilik asit polimerinin alt kritik çözelti sıcaklığının yapay sinir ağları ile tahmini*".