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Educational Background

Degree	Field	Institution	Year
Dr. rer. nat.	Computational Chemistry	University of Erlangen-Nürnberg, Germany Computer-Chemie-Centrum	2009
M.S.	Chemical Engineering	Hacettepe University, Turkey	2003
B.S.	Chemical Engineering	Hacettepe University, Turkey	2000

Academic Career

Designation	Institution	Year
Assistant Professor	Atılım University, Turkey Department of Chemical Engineering and Applied Chemistry	2013-present
Postdoctoral Research Associate	University of Texas at Austin, USA Institute for Theoretical Chemistry	2011-2013
Postdoctoral Research Associate	University of Hawaii at Manoa, USA W.M. Keck Research Laboratory in Astrochemistry	2009-2011
Research and Teaching Assistant	University of Erlangen-Nürnberg, Germany Computer-Chemie-Centrum	2004-2009
Research and Teaching Assistant	Hacettepe University, Turkey Chemical Engineering Department	2001-2004

Research Interests

Molecular modeling, computational chemistry.

Computational materials design.

Design and simulation of CO₂ absorption systems.

CO₂ capture.

Design, modeling and simulation studies of conductive polymers.

Modeling and simulation of process units in petrochemical plants.

Computational astrochemistry.

Simulation of the reactions between interstellar molecules and their reaction dynamics on icy grain mantles in the interstellar medium.

Extreme chemistry in ultra-cold environments.

Kuiper belt objects.

Vibronic interactions, Renner-Teller, Jahn-Teller and Pseudo Jahn-Teller effect on the structure, dynamics and spectra of molecules.

Chemical physics.

Parameterization of AM1* quantum mechanical, semiempirical method.

Organometallic and coordination chemistry.

Synthesis, characterization and modeling of stimuli-responsive polymers.

Artificial neural networks.

Projects Participated

The Scientific and Technological Research Council of Turkey (TUBITAK),
Investigation of reaction kinetics and mechanism of carbon dioxide capturing organic solvents by experimental and molecular modeling methods, Ankara, Turkey, March 2014- March 2016 (PI: E. Alper)

W.M. Keck Foundation, NASA Astrobiology Institute, and the University of Hawaii at Manoa, *Kuiper Belt Objects, Hawaii, USA, 2010-2011 (PIs: R.I. Kaiser and J.D. Head)*

German Research Foundation (DFG-Deutsche Forschungsgemeinschaft),
Parameterization of AMI for Redox-Active Metals, Erlangen, Germany, 2006-2009 (PI: T. Clark)*

The Scientific and Technological Research Council of Turkey (TUBITAK),
Prediction of lower critical solution temperature of N-isopropylacrylamide-acrylic acid copolymer by an artificial neural network model, Ankara, Turkey, 2002-2003 (PI: E. Alper)

Courses Taught

Introduction to Chemical Engineering
Chemical Process Calculations
Mass and Energy Balances in Engineering
Thermodynamics
Heat and Mass Transfer
Fluid Mechanics
Environmental Pollution
Chemical Computations
Chemical Engineering Design
Chemical Process Industries
Electrical Materials
Chemical Engineering Laboratory I-II

Publications

26. Ö. Y.-Orhan, H. Tankal, **H. Kayı**, E. Alper (2016), Investigation of a New Carbon Dioxide Capturing Organic Solvent: Reaction Mechanism and Kinetics, *Chemical Engineering & Technology*, Accepted.
25. B. Kaya, **H. Kayı** (2017), Design of novel tellurium and selenium containing semiconducting polymers using quantum mechanical tools, *Computational and Theoretical Chemistry*, 1099, pp. 45-54.
24. 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
23. Ö. Y.-Orhan, **H. Kayı**, E. Alper (Editor: Grammelis, Panagiotis) (2016), Kinetics of CO₂ capture by carbon dioxide binding organic liquids, *Energy, Transportation and Global Warming, Green Energy and Technology*, Springer International Publishing Switzerland, DOI 10.1007/978-3-319-30127-3_43, pp. 591-603
22. 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, *Turk J Chem*, DOI:10.3906/kim-1512-36
21. 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.
20. **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.
19. D. Nori-Shargh, N. Hasanzadeh, **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*, 26:547-554.
18. **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*, 20:2269.
17. 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*, 20:2249.

16. **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): 2549-2557.
15. 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.
13. **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*, 14:4942-4958.
12. **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.
11. **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.
10. **H. Kayı**, T. Clark (2011) AM1* parameters for palladium and silver. *Journal of Molecular Modeling*, 17:2585-2600.
9. **H. Kayı**, T. Clark (2010) AM1* parameters for manganese and iron. *Journal of Molecular Modeling*, 16:1109-1126.
8. **H. Kayı** (2010) AM1* parameters for gold. *Journal of Molecular Modeling*, 16:1029-1038.
7. **H. Kayı**, T. Clark (2010) AM1* parameters for cobalt and nickel. *Journal of Molecular Modeling*, 16:29-47.
6. **H. Kayı**, T. Clark (2009) AM1* parameters for vanadium and chromium. *Journal of Molecular Modeling*, 15:1253-1269.
5. **H. Kayı**, T. Clark (2009) AM1* parameters for bromine and iodine. *Journal of Molecular Modeling*, 15:295-308.

4. 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.

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

2. **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*, 11:55-60.

1. 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 Conference Proceedings

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

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

9. **Kayı, H**; Garcia-Fernandez, P; Bersuker, IB; Boggs, JE (2014) *Origin of Bending Instability of Small Linear Molecules and Deviations from Born-Oppenheimer Theory: pseudo Jahn-Teller Effect*, [25th Austin Symposium on Molecular Structure and Dynamics at Dallas](#), March 1-4, Dallas, Texas, USA, Lecture:10, Page 35

8. Head, JD; **Kayı, H**; Kaiser RI (2013) *Quantum chemical investigation of amino acid detection and formation in low temperature molecular ices typically present in the Outer Solar System*, [American Chemical Society, 245th ACS Meeting](#), April 7-13, New Orleans, USA, PHYS-292

7. **Kayı, H**; Bersuker, IB; Boggs, JE (2012) *The pseudo Jahn-Teller effect*, [XXIth International Symposium on the Jahn-Teller Effect](#), August 26-31, Tsukuba, Japan

6. **Kayı, H**; Kaiser, RI; Head JD (2011) *Theoretical investigation of the formation of the simple amino acids in extraterrestrial ices*, [American Chemical Society, Southwest Conference](#), November 9-12, Austin, Texas, USA

5. **Kayı, H**; Kaiser, RI; Head, JD (2010) *Theoretical investigation of the formation of the simple amino acid glycine and its isomers in extraterrestrial ices: Kuiper belt*

objects-laboratory studies, models, theory, and observations, [Pacifichem2010](#), December 15-20, **Honolulu, Hawaii, USA**, 1353

4. **Kayı, H**; Clark, T (2009) *Parameterization of AM1**, [Model\(l\)ing'09 Conference](#), September 6-11, **Erlangen, Germany**

3. **Kayı, H**; Clark, T (2008) *Parameterization of Bromine and Iodine for AM1**, [Darmstadt Molecular Modeling Workshop](#), April 29-30, **Erlangen, Germany**.

2. **Kayı, H**; Clark, T (2007) *Parameterization of Zinc for AM1**, [Darmstadt Molecular Modeling Workshop](#), May 15-16, **Erlangen, Germany**.

1. **Kayı, H**; Clark, T (2006) *Parameterization of Copper for AM1**, [Darmstadt Molecular Modeling Workshop](#), May 23-24, **Erlangen, Germany**.

National Conference Proceedings

7. Özkılınç, Ö; Kaya, B; **Kayı, H** (2016) *Design and simulation of novel semiconducting polymers for optoelectronic applications by quantum mechanical methods*. [12. National Chemical Engineering Congress UKMK-12](#), Aug 23-26, **İzmir**, pp. 648-653

6. Tankal, H; Yüksel-Orhan, Ö; Alper, E; Kayı, H (2015) *A DFT investigation of CO2 capture mechanism in TMBG 1-heksanol and 1-propanol solutions*, [6. National Air Pollution and Control Symposium, HKK 2015](#), Oct 07-09, **İzmir**

5. Tankal, H; Y.-Orhan, Ö; Alper, E; Özdoğan, T; **Kayı, H** (2015) *Quantum mechanical investigation of CO2 capture tendency of two organic solvents*, [5. National Physical Chemistry Congress](#), May 16-19, **Konya**, S30, page 40

4. Tankal, H; Y.-Orhan, Ö; Alper, E; **Kayı, H** (2015) *A DFT investigation of CO2 capture properties of organic solvents DBN and TBD inside 1-butanol and 1-propanol*, [2. National Computational Chemistry Congress](#), June 02-05, **Kars**, S04, page 10

3. **Kayı, H** (2014) *Computational chemistry and its applications*. [Amasya University, Mathematics Club and Physics Department - Invited Talk](#), Amasya

2. Bavbek, O; **Kayı, H**; Alper, E (2008) *Prediction of drying time in fluidized bed dryer by an artificial neural network model*, [UKMK-8](#), Aug 26-29, **Malatya**

1. **Kayı, H**; Elkamel, A; Alper, E (2002) *Prediction of lower critical solution temperature of N-isopropylacrylamide-acrylic acid copolymer*, [UKMK-5](#), September 2-5, **Ankara**

Journals Reviewed

Chemical Communications (Chem Comm)
Journal of Physical Chemistry A
Spectrochimica Acta Part A
Journal of Molecular Modeling
Journal of Applied Polymer Science
International Journal of Environment and Pollution
Environmental Engineering and Management Journal
E-Polymers Journal
Neural Computing and Applications
Canadian Journal of Chemistry
Journal of the Turkish Chemical Society: Chemical Engineering (JOTCSB)

International Collaborators

Ralf I. Kaiser (NASA Astrobiology Institute, UH, USA)
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Pablo Garcia-Fernandez (University of Cantabria, Santander, Spain)