

Prof. Viktorya Aviyente

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EDUCATION

Ph.D. in Chemistry	Boğaziçi University	1983
M.S.in Chemistry	Boğaziçi University	1977
B.S.in Chemistry	Boğaziçi University	1973
High School	Notre Dame de Sion French High School	1968

PROFESSIONAL APPOINTMENTS AND POSITIONS

Chemistry Teacher	Saint Benoit French High School	1973-1977
Teaching Assistant	Boğaziçi University	1977-1983
Assistant Professor	Boğaziçi University	1983-1988
Associate Professor	Boğaziçi University	1988-1995
Professor	Boğaziçi University	1995-2017
Emeritus Professor	Boğaziçi University	2017-present

ADMINISTRATIVE DUTIES

- Mentor of 65 graduate students (45 M.Sc., 20 Ph.D).
- Taught 18 undergraduate – 3 graduate courses
- Member of the Board of the Faculty of Arts and Sciences (2000-2009)
- Vice Head of the Chemistry Department (2000-2009)
- Head of the Chemistry Department (2009-2017).
- Head of Computational Sciences and Engineering Graduate Department (2006-2009).

TEACHING EXPERIENCE

CHEM 103	GENERAL CHEMISTRY I
CHEM 104	GENERAL CHEMISTRY II
CHEM 105	FUNDAMENTALS OF CHEMISTRY

CHEM 111	SURVEY OF CHEMISTRY I
CHEM 112	SURVEY OF CHEMISTRY II
CHEM 245	INORGANIC CHEMISTRY I
CHEM 261	COMPUTER APPLICATIONS IN CHEMISTRY
CHEM 331	INORGANIC CHEMISTRY II
CHEM 351	PHYSICAL CHEMISTRY I
CHEM 352	PHYSICAL CHEMISTRY II
CHEM 402	SEMINAR
CHEM 421	COMPUTATIONAL CHEMISTRY
CHEM 451	PHYSICAL CHEMISTRY III
CHEM 453	INTRODUCTION TO CHEMICAL KINETICS
CHEM 460	SYMMETRY IN CHEMISTRY
CHEM 473	RESEARCH TECHNIQUES IN CHEMISTRY (I)
CHEM 474	RESEARCH TECHNIQUES IN CHEMISTRY (II)
CHEM 475	RESEARCH TECHNIQUES IN CHEMISTRY (III)
CHEM 512	ADVANCED PHYSICAL CHEMISTRY
CHEM 522	ADVANCED COMPUTATIONAL CHEMISTRY
CHEM 556	STATISTICAL THERMODYNAMICS

RESEARCH TOPICS

The following topics are being investigated in the Aviyente research group with computational methods involving the use of hybrid quantum and classical mechanics:

- Determination of the effects of structure, catalyst and solvent effects on polymerization rates in free radical polymerization reactions of acrylate derivatives.
- Examination the stereoselectivity in organic reactions
- Modeling the deamidation reactions in peptides
- Modeling the inhibition/activation processes in enzymes
- Modelling mechanisms of removal of organic matter in wastewater
- Design of conductive materials for solar cells
- Effects of ionic liquids on hydrogenation reactions
- Design of potential drug molecules for photodynamic therapy
- Modeling of the catalytic properties of monoatomic metal catalysts

AWARDS AND GRANTS

- Grant from the Koç Foundation, 1979-1983.
- Kriton Curi Award to the best paper in BU, 1998.
Selçuki. C, Aviyente V., "Conformational Behaviour of 2-dimethylamino-1,3-dithiane in solution" *J. Chem. Soc. Perkin. Trans II*, 9,1835,1997.
- Best master thesis awarded to the mentee N.Senyurt (Boğaziçi University Research Fund), 1998.

“Computational Study of the Anomeric Effect in 2-[(4-substituted phenyl)seleno]-1,3-dithianes ”,

- Achievement Award in Research (Boğaziçi University Foundation) 2000.
- Best Ph.D. thesis award to the mentee B.Balta (Boğaziçi University Research Fund), 2003. “Analysis of the Structure, Fragmentation and Proton Exchange Mechanisms of Glycine and Diglycine”,
- Best Ph.D. thesis award to the mentee S.Catak (Boğaziçi University Research Fund), 2008." Elucidation of the Deamidation Mechanism of Asparaginy Residues in Peptides and Proteins ”,
- Best Ph.D. thesis award to the mentee N.Ç,Ölçüm (Boğaziçi University Research Fund), 2009, "Modeling the Selectivity in Pericyclic Reactions".
- Achievement Award in Research (Boğaziçi University Foundation) 2010.
- Best Ph.D thesis award to the mentee B.Ç.Dedeoğlu (Boğaziçi University Research Fund), 2016. "Modeling The Selectivity, Catalytic and Binding Effects in Organic Reactions and Protein Environment".
- Ranked among the 100 Turks Directing the Chemistry Science” in Turkey based on to the results of the “Golden Molecule”, 2022.

INTERNATIONAL GRANTS

- NATO Grant, 1996-1999.
- FIRCA (NIH) Grant, 2000-2003
- “COSBIOM” FP6-2004-ACC-SSA-2, 2005-2008 (member of the research group).
- British Council Grant, 2004. (“Setereoselectivity in Medicinal Chemistry”)

INTERNATIONAL COLLABORATIONS (2000 – present)

- G. Monard (Universite de Lorraine, Nancy I)
- A. Monari (Universite de Lorraine, Nancy I)
- M.F. Ruiz-Lopez (Universite de Lorraine, Nancy I)
- K. N. Houk (University of California at Los-Angeles)
- S. Arseniyadis (CNRS, Gif-sur-Yvette)
- C. Bolm (University of Aachen)
- P. Geerlings (VUB)
- F. De Proft (VUB)
- V. Veronique Van Speybroeck (Gent University)
- M. Waroquier (Gent University)
- I. Coldham (University of Sheffield)
- M. Feig (Michigan State University)
- I. Bahar (University of Pittsburg)
- C. Lifshitz (Hebrew University)
- D. Pasini (University of Pavia)

MEETINGS ATTENDED AND PRESENTATIONS (2017-present)

- 13th Chemical Physics Congress, 07-08 October 2022, Elazig “Modeling the Selectivity and Reactivity of Single site Catalysts”
- 258th ACS Meeting 25-29 August 2019 San Diego “A Computational Approach to Thermally Activated Delayed Fluorescence (TADF) Emitters in OLEDs”
- 12th Chemical Physics Congress, 12-13 October 2018, Safranbolu “Design and Degradation of Oligomers and Copolymers for Organic Photovoltaic Materials”
- Congress on 11th Electronic Structure: Principles and Applications 16-20 July 2018 Toledo “Rationalization of the Activity of the Lactone form of Topotecan towards the DNA/Topol Complex”
- SEPV 2018- Stability of Emerging Photovoltaics from Fundamental to Applications, Congress 20 - 23 February 2018 Barcelona “Design of Donor-Acceptor Copolymers for Organic Photovoltaic Materials: A Computational Study”
- 3rd Computational Chemistry Congress 12-14 October 2017, Ankara “Organik tepkime mekanizmalarına hesapsal yaklaşımlar”

THESIS SUPERVISED

- A. M.S.
1. Gökşin Apaydın (1993, Dr. UC Davis)
 2. Cenk Selçuki (1995, Dr. BU)
 3. Alimet Özen (1996, Dr. BU)
 4. Nurcan Şenyurt Tüzün (1997, Dr. BU)
 5. Ahu Akın (YL 1997, Dr. UIC)
 6. Bülent Balta (1998, Dr. BU)
 7. Dilek Duran (1999, Dr. BU)
 8. Şaron Çatak (1999, Dr. BU and U. of Lorraine)
 9. Kadir Diri (2001, Dr. U .Pittsburgh)
 10. Yeliz Aydeniz (2002)
 11. Hakan Günaydın (2003, Dr. UCLA)
 12. Seyhan Salman (2004, Dr. GATECH)

13. Cem Öztürk (2004, Dr. BU)
14. Derya Kut (2006)
15. İsa Değirmenci (2005, Dr. BU- Ghent U)
16. Mihriban İnçmen (2007)
17. Mehmed Zahid Ertem (2007, U. Minnesota)
18. İlke Uğur (2009, Dr. BU ve U. Lorraine)
19. Şeref Gül (2010, Dr. Koç U)
20. Tuğba Furuncuoğlu Özaltın (2010, Dr. BU)
21. Gülşah Cifci (2010, Dr. BU)
22. Sesil Agopcan (2011, Dr. BU)
23. Esra Bozkurt (2012, Dr. EFPL)
24. Berna Doğan (2012, Dr. Bahçeşehir U)
25. Aslı Yıldırım (2012, Dr. MSU)
26. Hasan Hüseyin İnce (2012)
27. Büşra Dereli (2013, Dr. Minnesota U)
28. Kumru Dikmenli (2015)
29. Gamze Bahadır (2016)
30. Taylan Turan (2017, Dr. Basel U)
31. Birce Kahraman (X- 2017)
32. Volkan Fındık (X- 2018)
33. Semiha Kevser Bali (X-2018)
34. Rengin Özek (X-2019)
35. Başak Koca (X-2019)
36. Beste Özaydın (X-2019)
37. Oğuzhan Kucur (X-2019)
38. Eyüp Metin (X-2019)
39. Cansu Kaynak (X-2019))
40. Deniz Ersoy (X-2019)
41. İpek Munar (X-2020)
42. Ekin Esmé Baş (X-2021)
43. Aylin Saltuk (X-2022)
44. İpek Azizoğlu (X-2022)
45. Melisa Kıran (X-2022)

X=co-advisor

B. Ph.D.

1. Prof. Dr. Safiye Erdem (1995) Marmara U
2. Prof. Dr. Cenk Selcuki (1999) Ege U
3. Doç. Dr. Feyza Atadinc Kolcu (2001) Çanakkale U
4. Prof.Dr. Aylin Sungur Konuklar (2002) ITU
5. Prof. Dr. Nurcan Şenyurt Tüzün (2002) ITU
6. Doç. Bülent Balta (2003) ITU
7. Dr. Dilek Duran (2003)
8. Prof. Dr. Alimet Özen (2004) Piri Reis U
9. Prof. Dr. Şaron Çatak (2007) BU
10. Dr. Kevser Göçmen Topal (2008) Tübitak
11. Prof. Dr. Nihan Çelebi Ölçüm (2009) Yeditepe U
12. Dr. İsa Değirmenci (2010) Samsun 19 Mayıs U

13. Dr. Özlem Karahan (2012)
14. Dr. Ilke Uğur (2014) METU
15. Dr. Burcu Çakır Dedeoğlu (2015) GTU
16. Dr. Tuğba Furuncuoğlu Özaltın (2016) Tüpraş
17. Dr. Sesil Agopcan Cinar (2017) Bilgi U
18. Dr. Gülşah Cifci Bağatır (2017)
19. Dr. Zeynep Pınar Haşlak (2019) Reims U
20. Dr. Deniz Akgül (2022)

PAPERS PUBLISHED IN THE LAST 5 YEARS (WOS 25.11.2022)

Number of publications 198
 Total number of citations 2637
 h-index 29

1	T. F. Özaltın, V. Aviyente, C., Atılgan, L., Demirel, 'Multiscale modeling of poly(2-isopropyl-2-oxazoline) chains in aqueous solution', <i>European Polymer Journal</i> , 88, 594–604, 2017
2	I. Uğur, S. Agopcan Cinar, B. Dedeoğlu, V. Aviyente, M. F. Hawthorne, P. Liu, F. Liu, K. N. Houk, and G. Jiménez-Osés, '1,3-Dipolar Cycloaddition Reactions of Low-Valent Rhodium and Iridium Complexes with Arylnitrile N-Oxides', <i>J. Org. Chem.</i> 2017 , 82, 5096–5101.
3	G. Çifçi, V. Aviyente, E. Demet Akten, G. Monard, 'Assessing protein-ligand binding modes with computational tools: the case of PDE4B', <i>J. Comput. Aided Mol. Des.</i> 2017 , 31, 563–575.
4	S. Agopcan Cinar, A. Ziylan-Yavaş, S. Catak, N. H. Ince, V. Aviyente, 'Hydroxyl radical-mediated degradation of diclofenac revisited: a computational approach to assessment of reaction mechanisms and by-products', <i>Environ. Sci. Pollut. Res.</i> 2017 , 24, 18458–18469.
5	Kilic, H.; Bayindir, S.; Erdogan, E.; et al. 'Bismuth nitrate-promoted disproportionative condensation of indoles with cyclohexanone: a new-type azafulvenium reactivity of indole' <i>NEW JOURNAL OF CHEMISTRY</i> , 2017 , 41, 9674-9687.
6	H. T. Turan, I. Yavuz, V. Aviyente, 'Understanding the Impact of Thiophene/Furan Substitution on Intrinsic Charge-Carrier Mobility', <i>JOURNAL OF PHYSICAL CHEMISTRY C</i> , 2017 , 121, 25682-25690.
7	H. T. Turan, O. Kucur, B. Kahraman, V. Aviyente, 'Design of donor-acceptor copolymers for organic photovoltaic materials: a computational study', <i>Physical Chemistry Chemical Physics</i> : PCCP, 2018 , 3581- 3591.
8	Z. P. Haslak, E. Bozkurt, B. Dutagaci, V. Aviyente, 'A DFT approach to discriminate the antagonist and partial agonist activity of ligands binding to the NMDA receptor', <i>MOLECULAR PHYSICS</i> , 2018 , 116, 323-337.
9	S. K. Bali, A. Marion, I. Uğur, S. Catak, V. Aviyente, 'Activity of Topotecan toward the DNA/Topoisomerase I Complex: A Theoretical Rationalization', <i>BIOCHEMISTRY</i> , 2018 , 57, 1542-1551.
10	D. H. Aydemir, G. Çifci, V. Aviyente, G. Boşgelmez-Tinaz, 'Quorum-sensing inhibitor potential of trans-anethole against <i>Pseudomonas aeruginosa</i> ', <i>Journal of Applied Microbiology</i> , 2018 , 125, 731-739.
11	N. Ferri, G. B. Ozaydin, A. Zeffiro, A. Nitti, V. Aviyente, D. Pasini, 'The efficient cyclopolymerization of silyl-tethered styrenic difunctional monomers', <i>JOURNAL OF POLYMER SCIENCE PART A-POLYMER CHEMISTRY</i> , 2018 , 56, 1593-1599.
12	T. F. Özaltın, S. Catak, B. Kiskan, Y. Yagci, V. Aviyente, 'Rationalizing the regioselectivity of cationic ring-opening polymerization of benzoxazines', <i>European Polymer Journal</i> 2018 , 105, 61-67.
13	V. Kocasoy, B. Dedeoğlu, O. Demir-Ordu and V. Aviyente, 'Influence of odd–even effect and intermolecular interactions in 2D molecular layers of bisamide Organogelators', <i>RSC Adv.</i> , 2018 , 8, 35195-35204.
14	V. Findık, I. Degirmenci, Ş. Catak, V. Aviyente, 'Theoretical investigation of thiol-ene click reactions: A DFT perspective', <i>European Polymer Journal</i> , 2019 , 110, 211–220.

15	D. Akgül, S. Agopcan Çinar, V. Aviyente, 'Role of ionic liquids on the selectivity and the rate of organic reactions: A computational approach', <i>Journal of Molecular Graphics and Modelling</i> , 2019 , 88, 309-317.
16	B. Koca, E. Hamuryudan, S. Catak, A. Erdogmus, A. Monari, V. Aviyente, 'Exploring the Photophysics of Polyfluorinated Phthalocyanine Derivatives as Potential Theranostic Agents', <i>Journal of Physical Chemistry C</i> , 2018 , 123, 24417-24425.
17	E. Arslan, B.S. Hekimoglu, S.A. Cinar, N. Ince, V. Aviyente, 'Hydroxyl Radical-Mediated Degradation of Salicylic Acid and Methyl Paraben: An Experimental and Computational Approach to Assess the Reaction Mechanisms', <i>Environmental Science and Pollution Research</i> , 2019 , 26, 33125-33134.
18	B. Koca, D. Akgul, V. Aviyente, 'Organocatalysts in Ring-Opening Polymerization: Revealing Their Effect on Stereochemistry', <i>European Polymer Journal</i> , 2019 , 109291.
19	G.B. Ozaydin, D. Avci, V. Aviyente, 'Binding of Self-Etching Monomers to Hydroxyapatite: A Computational Approach', <i>European Polymer Journal</i> , 2020 , 122, 109344.
20	Ö. N. Avci, S. Catak, B. Dereli, V. Aviyente, B. Dedeoglu 'ChemCatChem Elucidation of the Mechanism of Silver-Catalyzed Inverse Electron-Demand Diels-Alder (IEDDA) Reaction of 1,2-Diazines and Siloxy Alkynes', <i>ChemCatChem</i> 2020 , 12, 366–372.
21	O. Kucur, H. Taylan Turan, A. Monari, and V. Aviyente 'Computational Study of Photo-oxidative Degradation Mechanisms of Boron-Containing Oligothiophenes', <i>J. Phys. Chem. A</i> 2020 , 124, 1390–1398.
22	E. Arslan, B.K. Findik, V. Aviyente, 'A Blind SAMPL6 Challenge: Insight Into the Octanol-Water Partition Coefficients of Drug-Like Molecules via A DFT Approach', <i>Journal of Computer Aided Molecular Design</i> , 2020 , 34, 463-470
23	Z.P. Haslak, S. Agopcan Cinar, S. Sarigul Ozbek, G. Monard, I. Dogan, V. Aviyente, 'Elucidation of the atroposelectivity in the synthesis of axially chiral thiohydantoin derivatives', <i>Org. Biomol. Chem.</i> , 2020 , 18, 2233–2241.
24	I. Munar, V. Findik, I. Degirmenci, V. Aviyente 'Solvent Effects on Thiol-Ene Kinetics and Reactivity of Carbon and Sulfur Radicals' published as part of The Journal of Physical Chemistry virtual special issue "Paul Geerlings Festschrift", <i>J. Phys. Chem. A</i> 2020 , 124, 2580–2590.
24	E. E. Bas, S. Karahan, Z. Kostereli, M. Haktanir, V. Aviyente 'Pyrolysis of Alkanes: A Computational Approach', <i>J. Phys. Chem. A</i> 2020 , 124, 5700–5708.
25	E. Metin, N. Arsu, S. Catak, V. Aviyente 'Photophysical, kinetic and thermodynamic study of one-component Type II thioxanthone acetic acid photoinitiators', <i>European Polymer Journal</i> 2020 , 136, 109909.
26	S.F. Kurtoğlu, A.S. Hoffman, D. Akgül, M. Babucci, V. Aviyente, B. C. Gates, S. R. Bare, and A. Uzun 'Electronic Structure of Atomically Dispersed Supported Iridium Catalyst Controls Iridium Aggregation' <i>ACS Catalysis</i> , Articles ASAP (Letter), 2020 , 10, 12354-58.
27	A. Delgado, D. Sethio, I. Munar, V. Aviyente, E. Kraka, 'Local vibrational mode analysis of ion-solvent and solvent-solvent interactions for hydrated Ca ²⁺ clusters', <i>J. Chem. Phys.</i> 2020 , 153, 224303.
27	Z.P. Haslak, S. Zareb, I. Dogan, V. Aviyente, G. Monard, 'Using Atomic Charges to Describe the pKa of Carboxylic Acids', <i>J. Chem. Inf. Model.</i> 2021 , 61, 2733–2743.
28	A. Zıylan-Yavas, N. H. Ince, E. Ozon, E. Arslan, V. Aviyente, B. Savun-Hekimoglu, Aysen Erdinçler, <i>Journal of Computer-Aided Molecular Design</i> , 2021 , 35, 841–851.
30	V. Findik, B. K. Findik, V. Aviyente, A. Monari, 'Origins of the photoinitiation capacity of aromatic thiols as photoinitiators: a computational study', <i>Phys. Chem. Chem. Phys.</i> 2021 , 23, 24377-24385.
31	B. K. Findik, Z. P. Haslak, E. Arslan, V. Aviyente, 'SAMPL7 blind challenge: quantum-mechanical prediction of partition coefficients and acid dissociation constants for small drug-like molecules', <i>Journal of Computer-Aided Molecular Design</i> , 2021 , 35, 841–851.
32	Sule E. Gunal, I. Azizoglu, O. Arica, Z. P. Haslak, V. Aviyente, I. Dogan, 'Solvent dependent hindered rotation versus epimerization in axially chiral thiohydantoin derivatives: an experimental and a computational study', <i>Org. Biomol. Chem.</i> , 2022 , 20, 7622-7631.
33	Esra N. S., V. Findik, B. Dedeoglu, V. Aviyente, D. J. Tantillo, 'Theoretical Investigation of the Biogenetic Pathway for Formation of Antibacterial Indole Alkaloids from <i>Voacanga africana</i> ', <i>ACS Omega</i> 2022 , 7, 31591–31596.
34	P. Ulukan, E. E. Bas, R. B. Ozek, C. D. Kaynak, A. Monari, V. Aviyente, S. Catak 'Computational descriptor analysis on excited state behaviours of a series of TADF and non-TADF compounds', <i>Phys. Chem. Chem. Phys.</i> , 2022 , 24, 16167-16182.

35	D. Akgul, S. F. Kurtoglu-Oztulum, Y. Zhao, V. Findik, A. Monari, A. Uzun, V. Aviyente, 'Influence of ionic liquids on the electronic environment of atomically dispersed Ir on (MgO)(100)', <i>Physical Chemistry Chemical Physics</i> , 2022 , 24, 11305-11314
36	E. E. Bas, P. Ulukan, A. Monari, V. Aviyente, S. Catak, 'Photophysical Properties of Benzophenone-Based TADF Emitters in Relation to Their Molecular Structure', <i>J. Phys. Chem. A</i> 2022 , 126, 473-484.
37	B. K. Findik, U. Cilesiz, S. K. Bali, C. Atilgan, V. Aviyente, B. Dedeoglu "Investigation of iron release from the N- and C-lobes of human serum transferrin by quantum chemical calculations", <i>Org. Biomol. Chem.</i> , 2022 , 20, 8766-8774.