

# Ozge Ozkilinc

Udine, Italy

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## PERSONAL DATA

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PLACE AND DATE OF BIRTH: Ankara, Turkey | 30 June 1994  
NATIONALITY: Turkish  
LANGUAGES: Turkish mother tongue  
English, fluent  
Italian, basic  
ADDRESS: Università di Udine  
Via delle Scienze 206, 33100 - Udine, Italy.  
RESEARCHERID: [JMP-3810-2023](https://orcid.org/0000-0003-2023-339X)  
ORCID: [0000-0003-2023-339X](https://orcid.org/0000-0003-2023-339X)  
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## EDUCATION

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JAN 2022 - DEC 2024 Ph.D. in MATHEMATICAL AND PHYSICAL SCIENCES,  
Università degli Studi di Udine, Italy  
Thesis: Thermodynamic modelling and molecular dynamics simulations  
of deep eutectic solvents.  
Supervisor: Prof. Dr. Federico FOGOLARI

FEB 2018 - FEB 2021 M.Sc. in CHEMICAL ENGINEERING,  
Ankara University, Turkey  
Thesis: Investigation of the electronic band gap of benzothiazole-based  
donor-acceptor donor-type polymers by density functional theory.  
Supervisor: Assoc. Prof. Dr. Hakan KAYI  
GPA: 3.25/4

SEPT 2014 - JUN 2018 Minor Degree in INDUSTRIAL ENGINEERING,  
Atılım University, Turkey  
Faculty of Engineering (100% English)

SEPT 2012 - JUN 2017 B.Sc. in CHEMICAL ENGINEERING,  
Atılım University, Turkey  
Faculty of Engineering (100% English)  
GPA: 2.64/4

## SKILLS

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**Operating Systems:** *Experienced:* Linux | Windows

**Programming Languages:** *Experienced:* Python | Bash scripting  
*Familiar:* C++ | R

**Molecular Modeling & Simulations:** *Experienced:* GROMACS | AutoDock Vina | PyMOL |

Chimera | ORCA | Gaussian09 | COSMOtherm | MacMolPlt | Open Babel | VMD | TRAVIS  
*Familiar:* COMSOL | ASPEN | MATLAB

**High-Performance Computing:** User of national HPC resources

**Document Processing:** User of  $\LaTeX$ , OpenOffice, Microsoft Word

## FURTHER TRAINING & INTERNSHIPS

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- NOV 21-24, 2022 Workshop on Advancing Industrial Catalysis by Synergy of Experiments and Supercomputing Simulations.  
Bulgarian Academy of Sciences, Sofia, Bulgaria.
- JUL 17-28, 2022 CCP5 Summer School on Molecular Simulation Methods.  
Durham University, Durham, England.
- FEB 17-19, 2020 34th Molecular Modelling Workshop.  
Friedrich-Alexander-Universität, Erlangen, Nürnberg, Germany.
- JUL 7-8, 2019 Summer School on Advanced Electronic Structure Methods in Condensed Matter Physics.  
École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland.
- AUG 01-26, 2016 Internship in Production Department  
Drogsan Pharmaceuticals, Ankara, Turkey.  
-Examined the principles of drug production and raw materials according to GMP standards.
- JUL 01-30, 2015 Internship in Laboratory  
Republic of Turkey Ministry of Trade, Ankara, Turkey.  
-Determined the conformity of product samples in accordance with Customs-Trade Tariff Schedule using spectroscopic instruments.

## WORK EXPERIENCE

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- JAN 2022 - | Ph.D. Fellow  
DEC 2024 | at University of Udine, Italy  
granted by the Italian National Fellowship "National Operational Programme on Research and Innovation (PON RI 2014/2020 Asse IV Azione IV.5)".
- APR 2023 - | Doctoral Researcher (remotely)  
AUG 2024 | at eXactLab, Trieste, Italy  
supported by the University of Udine under research period.  
Project: *FAIRification of DES Simulation*.
- OCT 2023 - | Doctoral Visitor  
MAR 2024 | at University of Burgos, Spain  
supported by the University of Udine under research period.  
Project: *Design and Validation of Natural Deep Eutectic Solvents for the Removal of per/polyfluoroalkyl Substances from Contaminated Waters (NADESforPFAS)*.
- FEB 2018 - | M.Sc. Fellow  
FEB 2021 | at Ankara University, Turkey  
granted by the Turkish National Fellowship "The Scientific and Technological Research Council of Türkiye (TUBITAK Project No: 117Z354)".

## GRANTS

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- JAN 2022 PH.D. FELLOWSHIP  
(PON-Ministry of University and Research(MUR) Fellowship)  
University of Udine, Italy
- FEB 2018 M.SC. FELLOWSHIP  
(The Scientific and Technological Research Council of Türkiye(TUBITAK) Fellowship)  
Ankara University, Turkey

## MAIN HPC PROJECTS

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- JUNE 2024 - IS CRA Class C funding project, as PI  
MARCH 2025 76 800 stand. hours on Leonardo, CINECA, Italy.
- DEC 2023 - IS CRA Class C funding project, as COLLABORATOR  
SEP 2024 80 000 stand. hours on Leonardo, CINECA, Italy.
- OCT 2022 - IS CRA Class B funding project, as COLLABORATOR  
APR 2024 231 173 stand. hours on Marconi100, CINECA, Italy.

## PUBLICATION LISTS

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**WOS Citation Metrics:** h-index=3, 20 citations.

**Scopus:** h-index=3, 22 citations.

**Google Scholar Citation Metrics:** h-index=3, 26 citations.

## International Journals

1. **O. Ozkilinc**, M. A. Soler, P. Giannozzi, S. Aparicio, F. Fogolari. The Single-Parameter Bragg-Williams Model for Eutectic Solvents, *International Journal of Molecular Sciences*, vol. 26, no. 3, pp. 997, 2025. [Publisher: MDPI] <https://doi.org/10.3390/ijms26030997>
2. M. A. Soler, R. B. A. Yakout, **O. Ozkilinc**, P. Giannozzi, F. Fogolari. Blues\_cplx: Electrostatics at Protein-Protein and Protein-Ligand Interfaces, *Molecules*, vol. 30, no. 1, pp. 123, 2025. [Publisher: MDPI] <https://doi.org/10.3390/molecules30010159>
3. H. Kayı, E. Sen, **O. Ozkilinc**. Effect of chalcogen atoms on the electronic band gaps of the quinoxaline containing donor-acceptor-donor type semiconducting polymers: a systematic DFT investigation, *Journal of Molecular Modeling*, vol. 25, no. 5, pp. 123, 2019. [Publisher: Springer] <https://doi.org/10.1007/s00894-024-05985-2>
4. A. R. Buzatu, **O. Ozkilinc**, M. A. Soler, S. Fortuna, D. M. Dreava, I. Bitcan, V. Badea, P. Giannozzi, F. Fogolari, L. Gardossi. Reactive natural deep eutectic solvents increase selectivity and efficiency of lipase catalyzed esterification of carbohydrate polyols, *Catalysis Today*, vol. 426, pp. 114373, 2024. [Publisher: Elsevier] <https://doi.org/10.1016/j.cattod.2023.114373>
5. A. R. Buzatu, **O. Ozkilinc**, M. A. Soler, S. Fortuna, D. M. Dreava, I. Bitcan, P. Giannozzi, F. Fogolari, L. Gardossi, F. Peter. Lipase-catalysed esterification in a reactive natural deep eutectic solvent leads to lauroylcholine chloride rather than glucose ester, *Reaction Chemistry & Engineering*, vol. 9, no. 10, pp. 2623-2634, 2024. [Publisher: Royal Society of Chemistry] <https://doi.org/10.1039/D4RE00209A>
6. M. A. Soler, **O. Ozkilinc**, Y. Hunashal, P. Giannozzi, G. Esposito, F. Fogolari. Molecular electrostatics and pKa shifts calculations with the Generalized Born model. A tutorial

through examples with Blues2, *Computer Physics Communications*, vol. 287, pp. 108716, 2023. [Publisher: Elsevier] <https://doi.org/10.1016/j.cpc.2023.108716>

7. **O. Ozkilinc**, H. Kayi. Effect of chalcogen atoms on the electronic band gaps of donor-acceptor-donor type semiconducting polymers: A systematic DFT investigation, *Journal of Molecular Modeling*, vol. 25, no. 6, pp. 167, 2019. [Publisher: Springer] <https://doi.org/10.1007/s00894-019-4043-2>

## National Journals

1. H. Kayi, B. Kaya, **O. Özkılınç**. Design and Simulation of Semiconducting Polymers for Optoelectronic Applications by Using Quantum Mechanical Tools, *Journal of the Turkish Chemical Society, Section B: Chemical Engineering*, vol. 1, no. 1, pp. 1–12, 2016. [Publisher: Turkish Chemical Society] <https://dergipark.org.tr/en/pub/jotcsb/issue/28298/300648>

## PRESENTATIONS AT INTERNATIONAL CONFERENCES

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1. Ozge Ozkilinc (2024)  
*MDAnalysis User Group Meeting (UGM)*, King's College London, London, UK.  
“Exploring Lipase Biocatalysis in Sugar-Based Natural Deep Eutectic Solvents for Production of Novel Polymeric Compounds.”  
Oral Presentation.
2. Ozge Ozkilinc (2020)  
*34th Molecular Modeling Workshop (MMWS2020)*, Erlangen, Germany, February 17-19.  
“Effect of chalcogendiazole groups on the conductive properties of EDOT containing polymers” – Lecture No: 21.  
Oral Presentation.
3. Ozge Ozkilinc (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.
4. Ozge Ozkilinc (2018)  
*International Computational Science Congress (CSC-2018)*, Amasya, Turkiye, 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. Ozge Ozkilinc (2018)  
*12th Chemical Physics Congress (CPC-XII)*, Safranbolu, Turkiye, October 12-13.  
“Theoretical investigation of electronic properties of the ethylenedioxy-selenophene containing donor-acceptor-donor type conjugated polymer” – PP-32, Page 83.  
Poster Presentation.

## PRESENTATIONS AT NATIONAL CONFERENCES

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1. Ozge Ozkilinc (2018)  
*13th National Chemical Engineers Congress (UKMK2018)*, Van, Turkiye.  
“Bazi yeni oksadiazol iceren yariiletken polimerlerin DFT ile tasarimi ve simulasyonu (Design and simulation of some new oxadiazole containing semiconductor polymers by DFT)” – P87, Page 5830.  
Poster Presentation.

2. Ozge Ozkilinc (2017)  
*3rd Computational Chemistry Congress, Ankara, Turkiye.*  
*“Yogunluk fonksiyoneli teorisi yardimiyla bazi yariiletken polimerlerin tasarimi ve elektronik bant araliklarinin hesaplanmasi (Design and calculation of electronic band gaps of some semiconductor polymers with the help of density functional theory)” – Page 42.*  
Poster Presentation.

## PROFESSIONAL AND ACADEMIC EXPERIENCE

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- **Feb 2018 - Dec 202X:** UCTEA Chamber of Chemical Engineers Ankara Branch, 26th and 27th Term Board Member.
- **Sept 2016 - Jun 2017:** Atılım University Chemistry Society, Head of the Community.
- **Sept 2014 - Jun 2017:** UCTEA Chamber of Chemical Engineers Ankara Branch, Atılım University Student Representative.
- **Sept 2013 - Jun 2017:** Atılım University, Computational Chemistry Laboratory Project Student.
- **Jun 2013 - Jun 2017:** Atılım University Team Committee Member.
- **Oct 2012 - May 2013:** Atılım University Theater Society, “Run for Your Wife” (acting).

## AWARDS AND ACHIEVEMENTS

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- **2016-2017 Academic Year:** Atılım University 4th Rector’s Run Women Third Place Cup.
- **2016-2017 Academic Year:** Atılım University’s 50 Successful Students Certificate.
- **2014-2015 Academic Year:** Atılım University Sharing Success Certificate.

## REFERENCES

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- **Assoc. Prof. Dr. Federico Fogolari**  
Università degli Studi di Udine  
E-mail: federico.fogolari@uniud.it
- **Assoc. Prof. Dr. Hakan Kayi**  
Ankara University  
E-mail: hakan.kayi@ankara.edu.tr