Gözde Inis Demir

Date of birth: 27 Oct 1990 | **Nationality:** Turkish | **Phone number:**

(+49) 1752290791 (Mobile) | **Email address:** gozdeinis90@gmail.com |

Address: Bonn, Germany (Home)

WORK EXPERIENCE

12 FEB 2015 – 15 AUG 2022 Istanbul, Türkiye
HIGHER EDUCATION RESEARCH ASSISTANT INFORMATICS INSTITUTE OF ISTANBUL TECHNICAL UNIVERSITY

- Teaching Assistant
    - Hands-on sessions of the following lectures
        - Fundamental Software of Informatics (LINUX, Octave, Fortran, and Python)
        - Scientific Computing
        - Parallel Programming (MPI and OpenMP)
        - Object Oriented Programming (C/C++)
- Research Assistant
    - Software development for scientific purposes
        - Discovery of Energy Materials (Hydrogen and Ammonia Storage)
        - Development of a Framework for Force Field Generation
    - Automation of Workflows (on pre- and post-processing)
        - Preparation of inputs
        - Job submissions on HPC clusters
        - Analysis of the outputs of submitted jobs
- Webmaster of Computational Science and Engineering program

Department Computational Science and Engineering

1 FEB 2020 – 1 FEB 2023 Istanbul, Türkiye
SCHOLARSHIP HOLDER THE SCIENTIFIC AND TECHNOLOGICAL RESEARCH COUNCIL OF TURKEY

On a Project, namely "Computational Screening of Organic-Inorganic Hybrid Perovskites"
- Support for Software Development and Automation of Workflows
    - Extraction of features to be used in Machine Learning (ML)
    - Analysis of the results
    - Generation of ML models for the prediction of band gap (BG) and formation energy (FE) values
    - Identifying the promising perovskites by predicting BG and FE using generated ML Models

EDUCATION AND TRAINING

SEP 2008 – SEP 2013 Istanbul, Türkiye
BSC IN MATHEMATICS Istanbul Commerce University

Field of study Mathematics | **Final grade** 3.16

SEP 2014 – SEP 2017 Istanbul, Türkiye
MSC IN COMPUTATIONAL SCIENCE AND ENGINEERING Istanbul Technical University

Website https://itu.edu.tr/en/ | **Field of study** Computational Materials Science | **Final grade** 3.81 |

Thesis PyCASPESA: A new method for crystal structure prediction

SEP 2017 – CURRENT Istanbul, Türkiye
PHD IN COMPUTATIONAL SCIENCE AND ENGINEERING Istanbul Technical University

Website https://itu.edu.tr/en/ │ **Field of study** Computational Chemistry │ **Final grade** 3.91 │

Thesis Machine Learning Assisted Force Field Development for Nucleic Acids

LANGUAGE SKILLS

Mother tongue(s): **TURKISH**

Other language(s):

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken production	Spoken interaction	
ENGLISH	C1	C1	C1	C1	C1
GERMAN	A1	A2	A1	A1	A2

Levels: A1 and A2: Basic user; B1 and B2: Independent user; C1 and C2: Proficient user

DIGITAL SKILLS

Python │ Linux (Terminal Commands, Bash/Shell) │ Matlab │ GIT version control, Linux Command │ Modern Fortran │ Gnuplot │ Python visualization libraries (Matplotlib & Seaborn) │ Python DSci/ML Libraries (Numpy, Pandas, Sklearn, Scipy) │ Basic knowledge of Photoshop │ Basic knowledge of C │ Paralel Programming with MPI

ADDITIONAL INFORMATION

PUBLICATIONS

Crystal Structure Prediction and Dehydrogenation Mechanism of LiMg(BH4)3(NH3)2 – 2021
Inis Demir, G., Caputo, R., Demir, S., & Tekin, A.
The Journal of Physical Chemistry C, *125*(19), 10235-10242.

2D-FFCASP—A New Approach for 2D Structure Prediction Applied to Self-Assemblies of DNA Bases – 2022
Inis Demir, G., Demir, S., & Tekin, A.
Advanced Theory and Simulations, *5*(10), 2200308.

Stable and metastable crystal structures and ammonia dynamics in strontium chloride ammines – 2023
Demir, S., Inis Demir, G., Cankaya, M., & Tekin, A.
Submitted to Physical Chemistry Chemical Physics

NICE-FF: A Non-empirical, Intermolecular, Consistent, Extensible Force Field for Nucleic Acids and Beyond
– 2023
Inis Demir, G., & Tekin, A.
Submitted to Journal of Chemical Theory and Computation

HONOURS AND AWARDS

MAY 2022
EuroCC@Turkey Computhon 2022/1 – EuroCC Our team won the prizes in all three categories.
- Single-node: Parallel computation on multi-core CPUs.
- Single-node: Parallel computation on multiple GPUs.
- Multi-node: Distributed computing on multiple nodes + CPUs and GPUs

Links https://indico.truba.gov.tr/event/87/ │ https://twitter.com/EuroCC_Turkey/status/1525118043675828227?cxt=HHwWhoCxnfixp6oqAAAA

REFERENCES

Prof. Dr. Adem Tekin

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TUBİTAK Research Institute for Fundamental Sciences, Gebze, Kocaeli, Turkey
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