

Personal Information **Charalampos Trapalis, Dipl.-Ing., PhD**

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Summary An adaptable researcher seeking to improve and learn new skills. Main research interests include development of molecular dynamics (MD) forcefields and simulations of MD and coarse grain dynamics with a focus on small organic molecules at the interface with metallic substrates. Side interests include programming in Python and FORTRAN as well as setting up self-hosted home lab projects.

Work Experience

Jan 2021 – Dec 2022 **Research Assistant**
Mar 2018 – Jan 2019 Computational Materials Science Lab, University of Ioannina, Ioannina (Greece)
Dec 2016 – Jun 2017 **Projects: EKObuild, MUSICODE, CORNET, SMARTONICS**
Apr 2014 – Dec 2015 Developed two **backmapping algorithms** for regaining atomistic detail in active material regions. Implemented **coarse grained** potentials and **parametrized** existing **atomistic forcefield GAFF** for **small organic molecules** and **metal substrates**. **Developed procedures**, executed **simulations** and **analysis** for isomers of ICBA. Developed simulation protocols for the growth of molecular films on top of substrates and tools for the analysis of the resulting structures. Simulations performed on local **HPC** cluster. **Collecting, visualizing data** and **writing, submitting deliverables** for the aforementioned projects.
Heavy use of **BASH scripting** and **FORTRAN** for data parsing and analysis, including **OO features** of newer versions of FORTRAN, use of **C++** and **Python** for implementing various data management protocols during PhD.

2019 **Mandatory Army Service**

Other Experience

2014 – present **Programming Python/GTK+**
Developed an interface in **Python GTK+ 3.0** for syncing data between online services and an interface to an SQL database for collecting lists of tasks.

2016 – present **Home Lab**
Setting up **self-hosted servers** on **Linux** based machines.
More recently **raspberry pi** servers with **docker/podman** containers for Nextcloud, wordpress, Homeassistant, TT-RSS, pi-hole, Gitea with an nginx reverse proxy.

Mar 2014 – Jul 2017 **Lab Assistant (Teaching)**
Dept. of Material Science and Engineering, University of Ioannina, Ioannina (Greece)
Instructor during lab exercises for the FORTRAN and C++ classes.

Education

Jan 2014 – Dec 2018 **PhD in Materials Science and Engineering** Excellent
Dept. of Material Science and Engineering, University of Ioannina, Ioannina (Greece)
Thesis Title: Computational Study of Light Harvesting Materials for Applications in Organic Solar Cells.
Supervisors: Associate Professor D. G. Papageorgiou, Prof. E. Lidorikis, Prof. P. Patsalas.

Sep 2006 – Sep 2013 **Diploma of Materials Science and Engineering** 7.35/10
Dept. of Material Science and Engineering, University of Ioannina, Ioannina (Greece)
Dissertation Title: Properties of Oligo-thiophenes using Molecular Dynamics.
Supervisor: Associate Professor D. G. Papageorgiou.

Acquired Skills

| Experience Level | Elementary | Basic | Experienced |
|-----------------------|---|---|--|
| Languages | | | Greek: Mother Tongue, English: Excellent (Cambridge Proficiency in English (CPE)) |
| Computational Science | Merlin multidimensional optimization environment. MATLAB/Octave. C++/C | | FORTRAN, Python, BASH and TCL Scientific simulation tools: LAMMPS, NAMD Data Visualization: VMD, jMol, Avogadro, GNUplot Data analysis, manipulation: AmberTools, Open Babel, PackMol |
| Digital | GIMP/Inkscape, blender HTML/PHP Databases (SQL). | Python GTK+ 3.0 Docker/Podman Visual Studio Code | Windows and Linux systems. Office Suite LaTeX, git HPC software: TORQUE |
| Managerial | | | Mentoring skills gained as a guide for the thesis of 2 undergraduate students and 2 master students, and as a trainer during the initial training of a post-doctoral researcher and a PhD candidate. Organizational skills acquired from the collection and submission of deliverables for 3 European and one International projects and by participating in the organization of the XXXII Panhellenic Conference on Solid State Physics & Materials Science. Instructional skills acquired as an instructor in lab exercises performed for FORTRAN and C++ classes at the Department of Materials Science and Engineering. |

Academic Presence

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| Journals | Structural and Energetic Properties of P3HT and PCBM Monolayers on the Ag(111) Surface <i>Ch. Trapalis, E. Lidorikis and D. G. Papageorgiou</i> |
| Conferences | XXXII Panhellenic Conference on Solid State Physics & Materials Science 18-21 September 2016, Thessaloniki, Greece Poster: Molecular Modeling of the OPV Active Material at the Vicinity of Ag Nanoparticles <i>Ch. Trapalis, E Lidorikis, D. G. Papageorgiou</i> 10th International Symposium on Flexible Organic Electronics ISFOE15 6-9 July 2015, Thessaloniki, Greece Presentation: Molecular Modeling of Active Materials in the Vicinity of Ag Nanoparticles <i>Ch. Trapalis, E Lidorikis, D. G. Papageorgiou</i> 8th International Conference on Nanosciences & Nanotechnologies NN11 12-15 July 2011, Thessaloniki, Greece |
| Summer School | Graphene Summer School 2014 14-18 July 2014, Patras, Greece |

Additional Information

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| Memberships | Technical Chamber of Greece since October 2017 (Τεχνικό Επιμελητήριο Ελλάδας) |
| References | Associate Professor D. G. Papageorgiou University of Ioannina, 45110 Department of Materials Science and Engineering +30 26510 07373 dpapageo@uoi.gr Professor E. Lidorikis University of Ioannina, 45110 Department of Materials Science and Engineering +30 26510 07146 elidorik@uoi.gr |