MICHAEL MINOTAKIS

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EDUCATION

PhD in Physics — Oct 2019 - Sept 2023
Trinity College of Dublin — Dublin, Ireland
Project title: Design of novel magnetic materials by using Machine Learning and High-Throughput electronic structure methods.
Supervisor: Professor S. Sanvito

MSc in Materials Science and Technology — Nov 2016 - March 2019
University of Crete — Heraklion, Greece
Thesis title: First-Principle Simulations for low-dimensional Transition-Metal Dichalcogenide Alloys.
Supervisor: Professor I. N. Remediakis

BSc in Physics — Sept 2010 - June 2016
University of Crete — Heraklion, Greece
Thesis title: Density Functional Theory Calculations for 2-D Transition Metal Dichalcogenides Alloys.
Supervisor: Professor I. N. Remediakis

TECHNICAL SKILLS

Programming Languages	Python, SQL, Unix Bash-shell Scripting, Fortran
Software Packages	VASP, Quantum Espresso, LAMMPS, GPAW, Dacapo, Gaussian
Operating Systems	Linux, Microsoft Windows, Macintosh Operating System
Data Analysis	Pandas, Numpy, Scipy, Seaborn, BeautifulSoup, Matplotlib
Machine Learning	Scikit-Learn, Keras, Ridge Regression, Kernel Ridge Regression, Neural Networks
Miscellaneous	High Perfomance Computing, Git, MS Office, Open Office, LaTeX Matlab, Microcal Origin
Languages	Greek (Native), English (Fluent)

RESEARCH PROJECTS

Workflow for the Prediction of Ternary Phase Diagrams — Dublin, Ireland
Trinity College Dublin — Oct 2019 - Sept 2023

- Working in a team of two, we developed a workflow for predicting Ternary Phase Diagrams. The workflow was built in python with the use of various established in the community software packages (e.g. pymatgen, ASE etc).
- Trained surrogate models as energy predictors using state-of-the-art feature representations to assess material stability. Python APIs used to collect the data from well-established databases.
- Created suitable ternary materials candidates based on insights gained during the training process.
- A combination of machine learning and state-of-the-art *ab initio* software packages (VASP) was used in the project.
- Tested the robustness and the efficiency of the workflow and presented the results in fortnightly meetings with the rest of the group.
- The final workflow was used to find candidate stable alloys for the ternary systems of Ag-Au-Cu and W-Mo-Ta with results better than one of the community's standard databases. The results are anticipated to be published in two articles.
- Alongside with my colleague we presented two poster on the Psi-k community conference in Lausanne attended more than 1000 people, corresponding to the two parts of this work.

High-Throughput Study of the Antiferromagnetic Properties of Heusler Alloys. — Dublin, Ireland
Trinity College Dublin — Sept 2022 - Sept 2023

- Developed and executed a workflow to evaluate the stability and magnetic properties of a database consisting in over 900 Heusler compounds.
- The workflow was built on-top of well-established community tools (i.e. pymatgen, AFLOWLIB REST-API), along with state-of-the-art *ab initio* software packages (VASP).
- Expanded the search to include a variety of magnetic and structure configurations.
- The results are anticipated to be published in one journal article.

First-Principle simulations for the low-dimensional TMD alloys. Heraklion, Greece
University of Crete Jan 2018 - Jan 2019

- As part of my MSc thesis, used state-of-the-art *ab initio* software, Quantum-Espresso, to calculate the optoelectronic properties of transition metal dichalcogenide nanoribbons.
- The analysis of the results was performed using Python and Bash scripting. We utilized the high-performance computing cluster available at our university for the calculations.
- The results of our research were presented as part of my MSc thesis. Also presented as poster in two international conferences held on Herakion, which were attended by over 300 people each.

WORKING EXPERIENCE

Teaching Assistant 2022 - 2023
Trinity College Dublin *Dublin, Ireland*

- Responsible for preparing and delivering tutorials and marking assignments for the Maths II and Maths IV modules. Each class consisted of around 50 students, and I tailored the content of the classes to meet the specific needs of the students.
- Assisted in the Python laboratories for undergraduate physics students, providing support in understanding and completing exercises, such as solving the 1D Schrodinger equation with the Numerov algorithm.
- Worked as an assignment marker for the School of Physics laboratories, where I helped students understand the basics of error propagation and taught them how to analyze their data accurately.

Lead Educator 2019 - 2022
Trinity Walton Club *Dublin, Ireland*

- I was responsible for designing and delivering the Physics curriculum for the Trinity Walton Club. The aim of the club is to promote STEM subjects to teenagers in Ireland.
- I created a Physics curriculum inspired by applying the basics of dimensional analysis in order to understand the basics of kinematics. These classes were attended by around 30 students each time.

GRANTS

2019 **IRC Postgraduate Research Scholarship**, PhD funding for 4 years Ireland

2018 **State Scholarships Foundation MSc Research Scholarship**, MSc funding for 3 months. Greece

PUBLICATIONS

M. Minotakis, H. Rossignol, M. Cobelli, S. Sanvito. Machine learning surrogate model for acellerating the search of stable ternary alloys. https://doi.org/10.1103/PhysRevMaterials.7.093802

H. Rossignol, *M. Minotakis*, M. Cobelli, S. Sanvito. Machine learning assisted construction of ternary phase diagrams. https://arxiv.org/abs/2308.15907

M. Minotakis, S. Sanvito. High-throughput study of tetragonal and antiferromagnetic Heusler alloys. (in preparation)

REFERENCES

Prof Stefano Sanvito
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