





# THEODOROS PANAGIOTAKOPOULOS

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## LINKS







-  TheodorosPanagiotakopoulos.com
-  @Github
-  Theodoros Panagiotakopoulos
-  hackerrank

## EDUCATION

-  01/2019 - present PhD  
 University of Central Florida, Orlando  
**Artificial Intelligence Applications in Computational material science, GPA: 4/4**
-  09/2017 - 07/2019 Ms  
 National and Kapodistrian University of Athens, Athens  
**Nuclear and Particle Physics, Grade: 9.2/10, Valedictorian**
-  09/2011 - 07/2017 Bs  
 National and Kapodistrian University of Athens, Athens  
**Physics**

## SKILLS





### Programming

- Python/R 
- Julia 
- Bash 
- C/C++ 
- SQL 
- HTML 
- LaTeX 

### Operating Systems

- Linux 
- Windows 
- Mac OS 

### Software & Tools

- Machine Learning   
(Theano, TensorFlow, Keras, PyTorch, Scikit-learn, Flux)
- Data handling/analysis   
(numpy, scipy, pandas, statsmodels)
- Visualisation   
(matplotlib, gnuplot)
- Office/LibreOffice   
(Word, Excel, PowerPoint, OneNote, Outlook, Writer, Calc, Impress)

### Languages

- English 
- Greek 
- German 



## RELATIVE COURSES

- Probability Theory 1, 2
- Statistics 1, 2
- C/C++

## OBJECTIVE

Experienced **Ph.D.** in Applied Physics, adept in simulating and applying **AI/ML** for Computational Material Science, seeking a data science role to tackle complex challenges and drive impactful solutions.

## WORK HISTORY

-  08/2019 - present Graduate Research Assistant & Graduate Teaching Assistant  
 University of Central Florida, Orlando Florida

- NSF Projects**
  - Implemented **ML** and introduced a second-generation **neural-network** potential, significantly outpacing Density Functional Theory (DFT) in terms of speed and accuracy. This accomplishment played a pivotal role in securing renewed funding.
  - Created a fourth-generation **Neural Network** potential to overcome constraints in existing machine learning models, focusing on long-range charge transfer. This potential was adopted by our **data science** group, accelerating computational calculations.
  - Investigated the potential of graph Convolutional Neural Networks (GCNs) to enhance prediction accuracy, conducting experiments on truncated datasets, and analyzing predictions through parameter averaging from two datasets. This enhanced collaboration with the Department of Physics and Statistics in developing machine learning potentials.
  - Created a centralized **SQL database** by collating and organizing existing group member data from the server. Enhanced accessibility and facilitated result validation among team members, promoting seamless collaboration and data-driven decision-making.
- DOE Projects**
  - Performed **simulations, gathered, cleaned, and analyzed data** to examine the influence of ammonium cations on the Bi-catalyzed CO<sub>2</sub> Reduction Reaction, treating it as a classification problem.
  - Developed novel algorithms to compute CO<sub>2</sub> adsorption energy, resulting in data segmentation into two distinct regions. These advancements culminated in the calculation of electric forces and revealing the impact of cations on CO<sub>2</sub> adsorption.
  - Excelled in code **debugging and optimization** for Material Science applications, conducted **Linux-based HPC simulations**, and led advanced **software and methods** for **data analysis** to **predict** material properties.
  - Developed a custom Python library for material system design and analysis, fueling robust data science. Personally employed it for predictive machine learning in materials science.

## DATA SCIENCE AND CODING SKILLS

- Demonstrated excellence in **Python** and **R** for advanced coding and data analysis, harnessing these languages to extract valuable insights from intricate datasets.
- Skilled in **optimizing and recompiling C/C++** software to enhance performance for specific research and **computational needs**.
- Proficient in applying linear regression and Support Vector Machines (SVM) to enhance decision-making and optimize strategies within the context of **reinforcement learning**.
- Demonstrated proficiency in **training and testing Neural Networks** in **deep learning** to enhance data modeling and support well-informed decision-making.

- Proficient in utilizing ARIMA and SARIMA models to effectively analyze and forecast temporal data patterns, contributing to informed decision-making and accurate predictions in dynamic environments
- Showcased expertise in **data analytics** through numerous Ph.D. projects, skillfully extracting insights, making data-driven decisions, and delivering meaningful solutions.

## TECHNICAL SKILLS


- Exemplary knowledge of **data structures**, consistently designing and implementing efficient and optimized solutions for complex data-related challenges.
- Master (data integration) techniques with SQL, loading, extracting, and transforming data to ensure seamless and efficient processes.
- Expertise in **algorithm design** and **data science software architecture** for streamlined data workflows.
- Proficient in **high-performance computing cluster management**, specializing in **Slurm** for job scheduling, resource allocation, and **performance optimization**.
- Demonstrated **Git** expertise, maintaining organized code repositories for collaborative, data-driven projects.
- Proficiently creates compelling data visualizations with **Tableau**, **Matplotlib**, and **gnuplot** for clear communication of complex insights.


## MANAGEMENT & COMMUNICATION SKILLS


- **Supervising and independently completing projects**, consistently meeting budget and deadline goals with top-tier execution.
- Proficient in **conceptualizing, planning, and executing** end-to-end data science initiative aimed at solving critical business challenges.
- Successful in leading **diverse teams**, **fostering collaboration** and energizing **collective success**.
- Exceptional **communication and presentation skills**, bridging knowledge gaps and **ensuring clarity**.
- Excelled in **problem solving** and **analytical thinking** in dynamic evolving environments.
- **Excels in both written and verbal communication**, proficiently acquires knowledge and imparts insights with clarity.


## SELECTED - PUBLICATIONS

Electronic structure of cobalt valence tautomeric molecules in different environments


 **Theodoros Panagiotakopoulos**, Esha Mishra, Thilini K Ekanayaka, Duy Le, Talat Shahnaz Rahman, Ping Wang, Kayleigh McElveen, Jared Paul Phillips, Zaid Zaz, Saeed Yazdani, Alpha T. N'Diaye, Rebecca Y. Lai, Robert Streubel, Ruihua Cheng, Michael Shatruk and Peter A. Dowben


 2022


 Nanoscale


 [link](#)

Exploring Simulated Residential Spending Dynamics in Relation to Income Equality with the Entropy Trace of the Schelling Model


 **Theodoros Panagiotakopoulos**, George-Rafael Domenikos , Alexander V. Mantzaris


 2022


 MDPI


 [link](#)

Direct and indirect detection of dark matter


 **Theodoros Panagiotakopoulos**, Vasilios Spanos


 2019


 Pergamos library, National and Kapodistrian University of Athens


 [link](#)

Description of the method development for separating the Daliz from the normal  $\pi^0$  in the CDF detector

 **Theodoros Panagiotakopoulos**, Arkadios Manousakis

 2017

 Pergamos library, National and Kapodistrian University of Athens

 [link](#)