THEODOROS E. PANAGIOTAKOPOULOS

Theodoros.Panagiotakopoulos@ucf.edu | 321.202.3216 | teosfp@hotmail.com

LINKS

TheodorosPanagiotakopoulos.com
@Github
Theodoros Panagiotakopoulos

SKILLS

Programming

Python ●●●●●
Julia ●●●●●
Bash ●●●●●
LaTeX ●●●●●
R ●●●●○
SQL ●●●○○
C ●●●○○
HTML ●●●○○

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

- Condensed matter physics 1, 2
- Density Functional Theory
- Computational physics
- C/C++
- Experimental Methods for Physicists
- Electromagnetism 1, 2
- Quantum Mechanics 1, 2
- Statistical Mechanics 1, 2
- Statistics 1, 2

OBJECTIVE

Doctor (Ph.D.) in Engineering Physics, highly specialized in Artificial Intelligence Applications in Computational Material Science is seeking job where he can apply his data science, data engineering & machine learning problem solving skills, develop his leadership and make a great impact.

EDUCATION

01/2019 - present
University of Central Florida, Orlando — PhD
Artificial Intelligence Applications in Computational material science, GPA: 4/4

09/2017 - 07/2019
National and Kapodistrian University of Athens, Athens — Ms
Nuclear and Particle Physics, Grade: 9.2/10, I graduated first

09/2011 - 07/2017
National and Kapodistrian University of Athens, Athens — Bs
Physics

WORK HISTORY

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

- Continuing work towards a PhD in Computational Material Science
- **Introduced a second generation neural-network representation that is several orders of magnitude faster than Density Functional Theory (DFT)**. This method, relies on local properties and is not taking into account global changes in the electronic structure. This representation gives the energy and forces as a function of all atomic positions in systems of any size. An atomic **neural network** uses the local chemical environment to determine each atom's energy. A feed-forward **neural network**, in which information only passes in one direction toward the output layer, is the sort of **neural network** that is used for fitting energy. There are two layers: an input layer that feeds the network with the respective atomic positions and an output layer that holds the atomic potential energy. The regression is carried out by a number of intermediary hidden layers, with the number of layers and the number of neurons in each layer being empirically optimized for the particular application.
- **Developed a general solution for the limitations of current machine learning potentials by introducing a fourth-generation Neural Network, which is applicable to long-range charge transfer and multiple charge states**. It consists of highly accurate short-range atomic energies similar to those used in second generation **neural networks** potentials and charges determined from a charge equilibration method relying on electronegativities. Both, the short-range atomic energies as well as the electronegativities are expressed by atomic **neural networks** as a function of the chemical environments. For all these systems we demonstrate that fourth generation **neural network** potentials trained to DFT data are able to provide reliable energies, forces and charges in excellent agreement with electronic structure calculations. We show that previous generations of **neural network** potentials, which are unable to take distant structural changes into account, yield inaccurate energies and forces, which are correctly resolved by this **neural network** potential. These results apply to other types of machine learning potentials.

- **Worked with the Department of Statistics in order to research is and investigate how graph convolutional neural networks can enhance the accuracy of predictions**.The accuracy of predictions on a truncated dataset is examined in our experiments. The prediction made by averaging the parameters of two truncated datasets is then analyzed to determine if performance improvement can be observed. This is done by applying the methodological framework of the **Simplified Graph Convolutional Neural Network(SGC)** to Cora dataset. The impact of node removal on prediction accuracy is investigated by selecting nodes with three distinct patterns. Insights gained from these experiments shed light on which node patterns are crucial for optimizing the performance of **SGC**. If node removal is focused on a localized selection, the results demonstrate that **SGC** effectively utilizes the local information of network nodes. In this case, the applied method of improving the **SGC's** accuracy, has better performance compared to a case where the nodes were randomly dropped
- **Developed innovative numerical methods and algorithms for chemical potential calculations of metal on semiconductor junctions.** The model successfully predicts the formation of metallic clusters on the semiconductor surface, a result experimentally confirmed by scanning tunneling microscopy (STM) experiments at UC Davis. Moreover, the island areas grew linearly with time, exhibiting collective diffusion, and their total growth rate was inversely related to the temperature. Density Functional Theory simulations of the chemical potential and binding sites of the Pb/Ge(111) system were used to explain this nonclassical behavior of the system.
- **Introduced a novel method to model the electrolyte at the electrochemical interface using initio simulations of charge transfer processes at surfaces.** We presented a simple capacitor model of the interface that illuminates how to circumvent i) required large cell heights to reach convergence, which is a serious **computational cost** ii) the costly iterations calculations of reaction energetics to tune the surface charge to the desired potential. We derived a correction to the energy for finite cell heights to obtain the large cell energies at no additional **computational expense**. We furthermore demonstrated that the reaction energetics determined at constant charge are easily mapped to those at constant potential, which eliminates the need to apply iterative schemes to tune the system to a constant potential.
- **Investigated the cation effect using small quaternary ammonium cations with different sizes and symmetries.** For Bi-catalyzed CO_2 Reduction Reaction (CO_2RR) that produces CO and formate, density functional theory (DFT) calculations and ab initio molecular dynamics (AIMD) simulations were performed to examine the effect of asymmetric cations (such as $CH_3NH_3^+$) on CO_2 adsorption and activation. Experimental studies confirm that the asymmetric cations have a stronger promotional effect on the CO2RR activity than the symmetric ones, which is attributed to the asymmetric and weak hydration shell that stabilizes adsorbed CO_2. Moreover, by comparing the cations with different sizes (NH_4^+, Me_4N^+ and Et_4N^+), we observed a notable effect of the cation size on CO production activity, with a negligible impact on formate production. Our work further elucidates the critical effects of cation symmetry and size on CO_2RR and suggests a method to improve electrocatalysis with optimized electrolytes.
- Studied and reported the effect of creating an interface between a semiconducting polyaniline polymer or a polar poly-D-lysine molecular film and one of two valence tautomeric complexes, i.e., [CoIII(SQ)(Cat)(4-CN-py)2] ↔ [CoII(SQ)2(4-CN-py)2] and [CoIII(SQ)(Cat)(3-tpp)2] ↔ [CoII(SQ)2(3-tpp)2]. The electronic transitions and orbitals are identified using X-ray photoemission, X-ray absorption, inverse photoemission, and optical absorption spectroscopy measurements that are guided by density functional theory. Except for slightly modified binding energies and shifted orbital levels, the choice of the underlying substrate layer has little effect on the electronic structure. A prominent unoccupied ligand-to-metal charge transfer state exists in [CoIII(SQ)(Cat)(3-tpp)2] ↔ [CoII(SQ)2(3-tpp)2] that is virtually insensitive to the interface between the polymer and tautomeric complexes in the Co(II) high-spin state

- **Assist with compiling, debugging and optimization, of codes used in computational Material Science such as VASP, VASPsol and Quantum Espresso.** Perform, analyse and summarize validation simulations on **high-performance computer (HPC)** systems running **Linux.** Assist in the **implementation, development, and improvement of application software and methods** that can be utilized in **analyzing and interpreting data** in the physical sciences. **Four years active development of codes used in HPC**
- **Recently started coaching and supervising new coming graduate students to acclimate themselves within the group and execute their research project.** Provided **computational** help, assisted with class selection discussed with the advisor and group senior scientists about their research future steps. Keep abreast of new developments in **Computation Material Science** and be pro-active in introducing them to new graduate students. Help senior scientists with grant proposals by contributing sections of the proposal that describe the interplay between their research and **high-end computing resources.**
- **Instructor of introductory Physics 1 and 2.** Graduate and undergraduate electromagnetism and quantum mechanics. Design tutorials, and documentation for students in STEM field with the help and coordination of other university staff. **Leadership and mentorship** and instruction. **Authored manual with exercises and solution** for electromagnetism class. Recorded lectures and homework recitations for home and self study. Spearheaded review sessions and one to one consultations before the exams for struggling students. None of my students failed his exam.

10/2017 - 06/2019
National and Kapodistrian University of Athens, Athens Greece

Researcher & Graduate Student

- M.Sc in Physics: **Supersymmetric Models in Physics**. Athens 2019, Supervisor: Dr Vasilis Spanos. Studied Supersymmetry and applications in Particle Physics, Dark Matter, Cosmology and Condescend Matter Physics.

10/2011 - 06/2017
National and Kapodistrian University of Athens, Athens Greece

Researcher & Undergraduate Student

- B.Sc. in Physics: **Search for ultra rare π^0 decays with the CDF detector at Fermilab**. Athens 2017, Supervisor: Dr Arkadios Manousakis. Extensive simulations and statistical data analysis of elementary particle (π^0) decays and search via Dalitz plot (kinematical)analysis, for ultra rare decay modes.

DATA SCIENCE SKILLS

- Advanced proficiency in coding and data analysis using Python and R
- Unsupervised Learning: k-means clustering, principal component analysis
- Reinforcement Learning: linear regression, Support Vector Machines (SVM)
- Deep Learning. Neural Networks and decision trees.
- Time Series analysis: ARIMA SARIMA model

MATERIAL SCIENCE SKILLS

- Material simulation using ab initio Density Functional Theory (DFT) and molecular dynamics
- Expertise in surface visualization software packages (ASE, VESTA)
- Extensive use of VASP, VASPsol and Quantum Espresso software packages for novel material design.

MANAGEMENT AND COMMUNICATION SKILLS

- Manages projects with minimum supervision. Meets budgetary constraints and time deadlines
- Relates and collaborates well within a diverse team. Enthusiastic motivator
- Explains complex concepts to specialist and general audience
- Adapts and responds well to a rapidly changing environment
- A passionate learner with excellent verbal and written communication skills

AWARDS-FELLOWSHIPS

Spring 2022	Peer Tutoring Award	UCF Physics Dept.
2019-current	Research & Teaching Assistant Fellowship	UCF Physics Dept.

CONFERENCES-PRESENTATIONS

Spring 2022	American Physical Scociety	Chicago, Illinois.
Spring 2023	American Physical Scociety	Las Vegas, Nevada.
Spring 2023	STEM conference	Orlando, Florida.

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 π^0 in the CDF detector

Theodoros Panagiotakopoulos, Arkadios Manousakis

2017 Pergamos library, National and Kapodistrian University of Athens link

ARIMA model for Bitcoin price prediction

Theodoros Panagiotakopoulos

2023 Medium link

Randomly populated matrices

Theodoros Panagiotakopoulos

2023 Medium link

Simple Moving Average technique on the stock of the National Bank of Greece (NBG)

Theodoros Panagiotakopoulos

2023 Medium link