Theodoros Panagiotakopoulos

Curriculum Vitae

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Education

2019–present **Ph.D. in Computational Material Science**, GPA: 4/4, University of Central Florida (UCF), Orlando, Florida, USA

- **Ph.D. Thesis:** "*Modeling CO_2 Reduction Reaction on Bi(111) and understanding the growth of metallic islands on semiconductors*," under supervision of **Prof. Talat S. Rahman**

2017–2019 **M.Sc. in Nuclear and Particle Physics**, Grade: 8.8/10, National and Kapodistrian University of Athens, Athens, Greece. **I graduated first**

- **M.Sc. Thesis:** "*Direct and indirect detection of dark matter*," under supervision of **Prof. Vasilios Spanos**

2011-2017 **B.Sc. in Physics**, National and Kapodistrian University of Athens, Athens, Greece

- **B.Sc. Thesis:** "*Description of the method development for separating the Daliz from the normal π^0 in the CDF detector*," under supervision of **Prof. Arkadios Manousakis**

Advanced Courses Taken

Graduate Physics **Univercity of Central Florida, Orlando, Florida, USA**

- **Quantum mechanics 1:** Nouredine Zettili, book name: Quantum Mechanics Concepts and Applications, **grade: A**
- **Quantum mechanics 2:** J. J. Sakurai, book name: Modern Quantum Mechanics, **grade: A**
- **Electromagnetism 1:** Landau & Lifshitz, book name: The Classical Theory of Fields: Volume 2, **grade: A**
- **Electromagnetism 2:** Landau & Lifshitz, book name: Electrodynamics of Continuous Media: Volume 8, **grade: A**
- **Statistical Mechanics:** R. K. Pathria , book name: Statistical Mechanics, **grade: A**
- **Classical Mechanics:** Herbert Goldstein, book name: Classical Mechanics, **grade: A**
- **Condescend Matter Physics 1:** Steven M. Girvin, Kun Yang, book name: Modern Condensed Matter Physics, **grade: A**
- **Condescend Matter Physics 2:** Steven M. Girvin, Kun Yang, book name: Modern Condensed Matter Physics, **grade: A**

Graduate Physics

National and Kapodistrian University of Athens

- **Quantum mechanics:** Nouredine Zettili, book name: Quantum Mechanics Concepts and Applications, grade, **grade: 8/10**
- **Electromagnetism:** John David Jackson & Walter Greiner, book name Classical Electrodynamics & Classical Electrodynamics, **grade: 10/10**
- **String Theory:** David Tong, book name: David Tong Lectures on String Theory
- **Mathematical Physics**George B. Arfken, Hans J. Weber, Frank E. Harris & DeanG. Duffy , book name: Mathematical Methods for Physicists & Green's Functions with Applications, **grade: 9/10**
- **Particle physics:** Francis Halzen, Alan D. Martin & Günther Dissertori, IanG. Knowles, Michael Schmelling, book name: Quarks and Leptons & Quantum Chromodynamics (High Energy Experiments and Theory), **grade: 9/10**
- **Experimental methods for physicists:** Richard Fernow book name: Introduction to Experimental Particle Physics, **grade: 9/10**

Research Interests

- **Multi-scale modeling of chemical reactions and related phenomena at surfaces**
- **Density functional theory (D.F.T.)**
- **Surface Science**
- **Electronic Structure**
- **Catalysis**
- **Chemical Physics**
- **Molecular Structure**
- **Adsorption**
- **VASP**
- **Quantum Espresso**
- **Atomic Physics**
- **Quantum Physics**

PhD Thesis

Title	**Need to talk with my advisor for the Direct title**
Supervisor	**Talat S. Rahman.**
Find PhD Thesis	**to be updated**
Number of included citations	**more than 100, I will update the excact number**
Some information	**The first part of my research explores the influence of cations in the electrolyte on the electrochemical CO_2 reduction reaction (CO2RR). While previous studies focused on alkali metal cations, our work investigates a series of quaternary ammonium cations. We demonstrate that these non-metal cations have a significantly greater impact on CO_2 adsorption and CO2RR activity compared to their metal counterparts. According to computational studies, ammonium (NH_4^+) and methylammonium ($CH_3NH_3^+$) cations create a stronger bond between CO_2 and a bismuth (Bi) electrode compared to sodium (Na^+) cations. This enhanced binding is attributed to the electrostatic interactions between the cations and the adsorbed CO_2. The specific charge distribution and weak hydration shell of the ammonium-based cations are believed to be key factors in this phenomenon. Experiments validate our initial hypothesis: quaternary ammonium cations have a more pronounced stimulating effect on CO2RR compared to metal cations. Additionally, these experiments reveal a significant influence of both the specific type (identity) and concentration of the chosen cation on the production of carbon monoxide (CO). However, the effect on formate production appears to be minimal. Our findings suggest that while cation-stabilized CO_2 adsorption is crucial for CO production, it may not be as critical for formate formation during CO_2 reduction. The CO_2 work is supported by DOE Grant SC0024083** **The second part of my research is about the growth of single crystal metal islands on semiconductor surfaces which is important for technological process. In our joint experimental and theoretical examination of the growth of Pb on Ge(111), Low Energy Electron Microscopy (LEEM) measurements reveal an initial appearance of a Pb wetting layer until a critical coverage when nanocrystalline Pb islands abruptly form. Density functional theory based calculations find this critical coverage to be 1.33 ML, beyond which Pb atoms prefer to occupy the second layer. Ab initio thermodynamic calculations confirm that for Pb coverages below 1.33 ML the chemical potential of Pb (μ_{Pb}) in the wetting layer is less than that in bulk Pb, suggesting that Pb atoms prefer to be in the wetting layer, while at coverages higher than 1.33 ML the order is reversed implying that Pb atoms prefer to form bulk crystal, i.e. cluster. More interestingly, we find that at above 1.33 ML coverage, the μ_{Pb} in bilayer on Ge(111) is higher than that in bulk Pb, alluding that Pb atoms prefers to form a 3-d island, not a bilayer, in agreement with the LEEM observations that 3-d islands emerge suddenly out of the compressed wetting layer.**

Master Thesis

Title	**Direct and indirect detection of dark matter**
Supervisor	**Vasilios Spanos**
Find Master Thesis	**https://pergamos.lib.uoa.gr/uoa/dl/object/2878471**
Number of included citations	**58**
Some information	**It is an original material which I research and discover on my own. According to my master thesis, a brief reference is made to the standard model, the problem of the hierarchy is analyzed and reference is made to the way in which supersymmetry can respond to this problem. I then examine how the lightest supersymmetric particle (LSP), which is the main reason I have mentioned supersymmetry in the first chapter of my work, can be connected to dark matter. After the cross section for the scattering of the particles of the dark matter from ordinary matter is calculated, a detailed analysis of the direct dark mater detection modes is performed and analysis is made of the ways in which experiments that aim at dark matter detection work. Finally, indirect ways of detecting dark matter from annihi- lated dark matter particles to neutrinos and photons are examined. I allways compare theoretical predictions to data from observational astronomy in order to check the validity of the model which I am using**

Undergraduate Thesis

Title	**Description of the method development for separating the Daliz from the normal π^0 in the CDF detector**
Supervisor	**Arkadios Manousakis.**
Find undergraduate Thesis	**https://pergamos.lib.uoa.gr/uoa/dl/frontend/el/browse/1668201**
Number of included citations	**11**
Some information	**It was based on research paper that has been produced by other researchers. I had to study it, reproduce it and piece it an origi- nal presentation. According to my undergraduate thesis, reference is made not only to the decomposition reactions of π^0 but also to the probability that occurs in each of them. A study is also made to a detailed analysis of the structure and mode of operation of the Tevatron accelerator and of the CDF (Collider Detector at Fermi- lab), SVXII, ISL (Silicon Layers) and COT (Central Outer Tracker) detectors, which are the trace detection systems and are designed to detect the charged particle trajectories. Next, the conversion of $\gamma \rightarrow e^- e+$ to Tevatron is studied to reduce the uncertainty in the initial conversion probability. The above procedure is done by creating an algorithm. From the reconstruction of the mass of π^0 and from the combination of the four trajectories, I find the cleavage position of π^0 . Then we analyze the possibility of using the space variables in the decomposition of π^0 while analyzing the topology of both normal and Daliz π^0 . After the study we come to the selection of the appro- priate variables which are defined as firstpoint and minpoint, where Monte Carlo technic plaid a crucial role. Finally, from the diagram that emerged from the breakpoints of π^0 , we proceeded to identify the ISL, COT and SVXII detectors**

Research Experience

2019 - now **Research Assistant**, **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. **(Paper submitted in Nature Communications. One of the top in Nation)**

Research Assistant, **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.,** $[Co^{III}(SQ)(Cat)(4-CN-py)_2] \rightleftharpoons [Co^{II}(SQ)_2(4-CN-py)_2]$ **and** $[Co^{III}(SQ)(Cat)(3-tpp)_2] \rightleftharpoons [Co^{II}(SQ)_2(3-tpp)_2]$**.** 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 $[Co^{III}(SQ)(Cat)(3-tpp)_2] \rightleftharpoons [Co^{II}(SQ)_2(3-tpp)_2]$ that is virtually insensitive to the interface between the polymer and tautomeric complexes in the Co(II) high-spin state. **(Paper Published in Nanoscale. Considered high impact journal)**

Research Assistant, **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. **(Needs to be published. Draft is ready.)**

Research Assistant, In collaboration with researchers at Bochum, Germany, we investigated the behavior of single molecules, a key factor in tuning their physical properties, such as reactivity. One important application for large, bulky molecules is the activation of smaller molecules. The class of extremely reactive, electron-rich phosphines holds promise as capture molecules, for example, for carbon dioxide (CO_2) by forming zwitterionic Lewis base adducts. Tris(tetramethylguanidinyl) phosphine ($P(tmg)_3$) shows the greatest potential for future use due to its high synthesis yield from inexpensive and commercially available bulk precursors. We employed a combination of low-temperature scanning tunneling microscopy and density functional theory calculations to unravel the structure and adsorption geometry of a bulky, flexible $P(tmg)_3$ molecule on Ag(100). We also discuss the influence of adsorption on the reactivity of $P(tmg)_3$. Furthermore, we investigated the adsorption geometry of $P(tmg)_3$ dimers, which are the thermodynamically preferred formation on Ag(100). The influence of dimerization on the molecular properties is also discussed. By understanding the interaction between the superbasic phosphine and the metal surface, combined with the easy accessibility of $P(tmg)_3$, we anticipate that electron-rich phosphines on surfaces will find widespread use in small molecule activation.**We are writing the paper**

Research Assistant, **Collaborated with the Department of Statistics** and explored the Schelling model of segregation, which has provided researchers with a simple model to explore residential dynamics and their implications upon the spatial distribution of resident identities. Due to the simplicity of the model, many modifications and extensions have been produced to capture different aspects of the decision process taken when residents change locations. Research has also involved examining different metrics for track segregation along the trace of the simulation states. Recent work has investigated monitoring the simulation by estimating the entropy of the states along the simulation, which offers a macroscopic perspective. Drawing inspiration from empirical studies which indicate that financial status can affect segregation, a dual dynamic for movements based on identity and financial capital has been produced so that the expenditure of a monetary value occurs during residential movements. Previous work has only considered a single approach for this dynamic and the results for different approaches are explored. The results show that the definition of the expenditure dynamic has a large effect on the entropy traces and financial homogeneity. The design choice provides insight for how the housing market can drive inequality or equality. **Paper published at MDPI**

Instructor of introductory Physics 1 and 2, Taught graduate and undergraduate electromagnetism and quantum mechanics. Designed tutorials and documentation for students in STEM fields with the help and coordination of other university staff. Provided **leadership and mentorship** and instruction. Authored manuals with exercises and solutions for electromagnetism class. Recorded lectures and homework recitations for home and self-study. Organized review sessions and one-to-one consultations before exams for struggling students. None of my students failed their exams.

2018 - 2019 **Teaching Assistant: Physics 1 (assistant of Dr. Manousakis Arkadios)**, National and Kapodistrian University of Athens, Athens, Greece

2018 - 2019 **Grader: Physics 1 (assistant of Dr. Manousakis Arkadios)**, National and Kapodistrian University of Athens, Athens, Greece

2018 - 2019 **Teaching Assistant: Physics 1 (assistant of Dr. Manousakis Arkadios)**, National and Kapodistrian University of Athens, Athens, Greece

2017 - 2018 **Teaching Assistant: Physics 1 (assistant of Dr. Manousakis Arkadios)**, National and Kapodistrian University of Athens, Athens, Greece

2016 - 2017 **Teaching Assistant: Physics 1 (assistant of Dr. Manousakis Arkadios)**, National and Kapodistrian University of Athens, Athens, Greece

2016 - 2017 **Grader: Physics 1 (assistant of Dr. Manousakis Arkadios)**, National and Kapodistrian University of Athens, Athens, Greece

2011 - 2019 **Private Tutor**

Coding Languages

- Python

Computer Skils

- UBUNTU
- WINDOWS

Competitions I participated in

1/4/2021 **Qualifiers exams in Phyisics**, University of Central Florida, Orlando, Florida, USA

11/28/2009 **Pan-Hellenic Student Competition of the 8th European Olympiad of Sciences EUSO 2010**

3/6/2010 **20th Panhellenic Student Physics Competition**

1/23/2010 **Efklidis, Mathematical Competition, Qualifying examinations for the Hellenic Mathimaticl Olimpiade**, Helenic Mathematical Society

1/17/2010 **Efklidis, Mathematical Competition, Qualifying examinations for the Hellenic Mathimaticl Olimpiade**, Helenic Mathematical Society

11/21/2009 **Thalis, Mathematical Competition (Successfully passed)**, Helenic Mathematical Society

11/1/2009 **Thalis, Mathematical Competition**, Helenic Mathematical Society (Successfully passed)

Presentations - POSTERS

11/04/2023 **Efficacy of non-metallic cations in electrochemical CO2 reduction on Bi (111) electrode: a first principles study.**, APS March Meeting 2024 Minneapolis

11/04/2023 **First principles study of CO_2 electroreduction on Bi(111) electrode: Effect of metallic and non-metallic cations** , ASEMLF Conference Orlando Florida

03/04/2023 **Stabilization of CO_2 adsorption on Bi(111) electrode in electrochemical environment using non-metallic cations: A first principles study.** , STEM Conference Orlando Florida

03/04/2023 **Stabilization of CO_2 adsorption on Bi(111) electrode in electrochemical environment using non-metallic cations: A first principles study.** , APS March Meeting 2023, Las Vegas

03/16/2022 **Understanding the growth of Pb on Ge(111): a first principles study**, APS March Meeting 2022 Chicago

Seminars

- Lectures on Science in Confinement- From Surface Science to Nanoscience to 2D, Univercity of Central Florida & Max Planck Institute, USA & Germany
- Distinguished Lecture Series on Catalysis Univercity of Central Florida, Orlando, Florida, USA

Mathematics /Physics schools

7/25/2010 - 7/31/2010 **Fourth Mathematical summer school at Leptokria Pieria Greece**, Hellenic Mathematical Society, Athens, Greece

2/25/2010 **Sixth international particle physics Masterclasses at National and Technical University of Athens**, National and Technical University of Athens, Athens, Greece

7/25/2010- 7/31/2010 **Fourth Mathematical summer school at Leptokria Pieria Greece**, *Hellenic Mathematical Society, Athens, Greece*

Fellowsinps and Awards

- Peer Tutoring Award UCF Physics Dept.
- Research & Teaching Assistant Fellowship UCF Physics Dept.
- DCOMP award, American Physical Society, 2024

Languages

- **English C2** City and Guilds
- **English B2** Cambridge
- **English B2** City and Guilds
- **German B1** Goethe

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]