SOCIETY OF PHYSICS STUDENTS
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SPS Chapter Research Award Proposal

Project Proposal Title	Density Functional Theory Calculations for Van der Waals Material Candidate
Name of School	University of Central Florida
SPS Chapter Number	1076
Total Amount Requested	$2000

Abstract

At the University of Central Florida, the characterization of quantum materials is a prominent research field. Before physical experiments are performed, Density Functional Theory is applied to understand their band structure. We seek to build a computer to handle DFT simulations to independently study $MoPS_3$, a Transition Metal Phosphorous Trichalcogenide.

Proposal Statement

Overview of Proposed Project

Research Question:

What can Density Functional Theory tell us about the electronic structure of $MoPS_3$?

Motivation, Description, and Goals:

At UCF, many research groups are focused on the characterization of quantum materials. My (Zakaria El-Helw) research group specifically focuses on Angle-Resolved Photoemission Spectroscopy (ARPES) studies of topological insulators and other quantum materials. Since we focus on ARPES, we need to outsource initial theoretical calculations to other groups that specialize in Density Functional Theory (DFT) before we continue our own studies.

As undergraduate students, these techniques are fascinating to us, but the amount of outsourced work to begin a new study slows down research time, which graduate students can afford as their participation in this research can span anywhere from 4-7 years, whereas our involvement is limited to 2-3 years before the graduate school application cycle. With this in mind, the difference between a DFT study taking a few weeks and staying within our purview and the same study taking a few months, relaying between two different institutions, is significant. Furthermore, the scope of topics that we can explore is limited by the significant costs of either computation time at a local cluster, or the aforementioned outsourcing. As we would like to study a new group of materials, and are all undergraduates, we would like to make further experimental studies as easily approvable as possible, something which can be achieved by cutting down initial costs.

SPS Connection:

This research project will develop the capacity for undergraduates to more autonomously explore the field of condensed matter by allowing them to interact and understand with the calculations needed to begin a study of a material, and to empower them to take that process into their own hands, developing their own research. The establishment of this dynamic within the undergraduate program for those interested in materials will serve to improve outcomes for physics students by allowing them to contribute to the body of science, which falls in line with SPS's stated goal of helping students flourish professionally.

Background for Proposed Project

Transition Metal Phosphorous Trichalcogenides (TMPTs) are a class of van der Waals materials with insulating properties. Van der Waals materials are remarkable for their layered structures, enabling exfoliation into two-dimensional crystals. Their applications extend to spintronics, catalysis and energy storage. There have been studies of other TMPTs including $PtPS_3$ and $PdPS_3$[1] using DFT, as well as $FePS_3$[2].

The material we'd like to study is $MoPS_3$, a TMPT. Molybdenum has attracted much attention due to its interesting properties in related materials, chiefly MoS_2, a Transition Metal Dichalcogenide, wherein unique electronic and optical properties have been discovered, suggesting $MoPS_3$ may host similarly novel phenomena.

To characterize $MoPS_3$, we will employ Density Functional Theory (DFT). DFT is the standard computational method for materials characterization, offering an optimal balance between accuracy and computational cost. Its efficiency allows for the simulation of realistically large systems while avoiding the expense of higher-level methods like Quantum Monte Carlo (QMC) or Many-Body Perturbation Theory (MBPT). Furthermore, as a first-principles method, DFT does not require pre-existing experimental data or empirical parameter-fitting, which would be necessary for simpler, faster methods like tight-binding models. We acknowledge DFT's known limitations, such as its tendency to underestimate band gaps and its difficulties with strongly correlated systems. However, its balance of predictive power and efficiency makes it the optimal choice for this project.

DFT avoids complex many-body computations by solving the Kohn-Sham equations. These describe a fictitious system of non-interacting electrons moving in an effective potential, which is constructed to yield the same ground-state density as the real material. Since this effective potential itself depends on the electron density, solving these equations requires a self-consistent field (SCF) loop. This iterative process yields the final ground-state electron density, from which all other required properties can be derived.[3]

Expected Results

We expect to characterize $MoPS_3$ as a layered van der Waals semiconductor, identifying its magnetic ordering, band gap, and spin-orbit effects. Calculations will reveal whether Dirac-like dispersions or valley features emerge in monolayer form, clarifying its potential as a novel 2D quantum material with exotic electronic properties.

Description of Proposed Research - Methods, Design, and Procedures

Our central aim is to determine whether $MoPS_3$ hosts Dirac cones, valley features, or other exotic band phenomena arising from its layered van der Waals lattice and 4d molybdenum orbitals.

We will employ Density Functional Theory (DFT) using Quantum ESPRESSO on a Debian-based workstation with 16 CPU cores and 128 GB memory. Calculations will begin with structural optimization of bulk and monolayer $MoPS_3$, followed by electronic band structure and density of states analysis. Spin-polarized and spin-orbit coupling (SOC) calculations will be performed to capture magnetic ordering and band splitting.

We will compare results across GGA, GGA+U, and hybrid functionals, and use supercell models to explore strain and defects. This integrated approach will provide the first comprehensive characterization of $MoPS_3$, clarifying its potential as a novel 2D quantum material.

Plan for Carrying Out Proposed Project

Personnel and Expertise:

Zakaria El-Helw

- Project lead
- 1 year of experience in researching quantum materials using ARPES and DFT data
- Secretary of UCF SPS Chapter

Andres Gualdron

- 4 months of experience in theoretical condensed matter research using computational methods
- Experienced in computer assembly and repair
- SPS Member

Alexander Dorn

- 2 years of experience in mathematical physics research
    - Differential Geometry
    - Algebraic Topology
- Experienced in computer assembly and repair
- Vice President of UCF SPS Chapter

James Jackson

- 4 months experience in modelling condensed matter behavior using partial differential equations
- SPS Member

We invite other UCF SPS members to contribute to the project.

Research Space

At UCF, physics undergraduates have a room for research and academic collaboration. It is secure as it is locked, requiring card access to enter.

Contributions of faculty advisors or the department

Milo Sprague (Graduate student)

- General advisor
- Experienced in ARPES, ran DFT in the past, familiar with the software, processes and theory.

Dr. Madhab Neupane (Professor of physics)

- General advisor

Dr. Paulo De Faria Jr. (Professor of physics)

- General advisor

Dr. Aniket Bhattacharya (Professor of physics)

- SPS Advisor

Project Timeline

Late January 2026

- Receive funding
- Purchase parts

Mid-late February 2026

- Receive parts
- Build computer
- Set up operating system
    - Debian
- Set up software
    - Quantum ESPRESSO
    - Burai

Early-mid March

- Run simulations of well known, related materials on the system (WSe_2, $FePS_3$, MoS_2, etc.)
    - Benchmark system
- Familiarize team members with the software and simulation methods
- Run DFT simulation on $MoPS_3$
    - Preliminary data analysis

Mid-late March: APS, Spring Break, Midterm season

Early-mid April

- Analyze last DFT run
    - Run again if needed
- Put together models of band structure/fermi surface
- Begin summarizing findings
- Begin writing report

Late April-early May: Finals

Mid-late May:

- Finish and submit interim report (May 31st)
- Begin writing final report and paper

June-August: REUs, Summer Internships

Mid-late August

- Paper writing
- Review with advisors

September

- Finish paper
- Submit final report

Budget Justification

CPU: AMD Ryzen 9 7950X 4.5 GHz 16-Core Processor ($501.00 @ B&H)

- DFT is an incredibly CPU-Heavy Process, the speed of the CPU will directly impact the performance of the calculations done.

CPU Cooler: be quiet! Pure Rock Pro 3 Black 120mm Rifle CPU Cooler ($59.90 @ Newegg)

- Since the calculations are entirely handled by the CPU a good cooler is essential to keep the processor at an optimal temperature and avoid underperformance or in the worst case CPU damage.

Motherboard: MSI X670E GAMING PLUS WIFI ATX AM5 Motherboard ($189.99 @ Amazon)

- The motherboard will hold all of the components and communicate them, although the motherboard choice doesn't necessarily affect performance it must be reliable to avoid catastrophic failures.

Memory: Corsair Vengeance 128 GB (2 x 64 GB) DDR5-6400 CL40 Memory ($704.00 @ Newegg)

- This is the most important part, since HPC CPUs with more memory channels are too expensive, getting a high quality RAM with the highest available speed will compensate for the fewer channels.
- The 2 x 64 configuration is more efficient for AMD Processors, which will further improve the performance

Storage: Samsung 990 Pro 2 TB M.2-2280 PCIe 4.0 X4 NVME Solid State Drive ($179.68 @ Amazon)

- During the calculations massive amounts of read and write operations will be performed, for this reason a high performance storage solution is essential to avoid bottlenecking the calculations.

Power Supply: Corsair RM850x SHIFT 850 W 80+ Gold Certified Fully Modular Side Interface ATX Power Supply ($134.99 @ Newegg)

- The power supply (PSU) is responsible for delivering power to all components, a good PSU (rating 80+ gold) is necessary to avoid power fluctuations that might impact performance or jeopardize the entire computational process. Furthermore, the system is expected to run from a few hours to entire days, therefore a higher wattage PSU is necessary for safety reasons.

Case: Fractal Design Pop Air ATX Mid Tower Case ($84.99 @ B&H)

- High quality housing for components

+$145.45 in case of market fluctuations or unexpected associated costs

Total: $2000

Other contributions:

The Physics Department has an uninterruptible power supply (UPS) that we have access to, it will be a safety measure to handle the event of a power surge or outing.

Bibliography

1. Sugita, Y., Miyake, T., Motome, Y., Multiple Dirac Cones and Topological Magnetism in Honeycomb-Monolayer Transition Metal Trichalcogenides. Phys. Rev. B 97, 035125 (2018). https://doi.org/10.48550/arXiv.1704.00318

2. Ilyas, B., Luo, T., von Hoegen, A. et al. Terahertz field-induced metastable magnetization near criticality in FePS3. Nature 636, 609–614 (2024). https://doi.org/10.1038/s41586-024-08226-x

3. Eugene S. Kryachko, Eduardo V. Ludeña, Density functional theory: Foundations reviewed, Physics Reports, Volume 544, Issue 2, 2014, Pages 123-239, ISSN 0370-1573, https://doi.org/10.1016/j.physrep.2014.06.002