InP Quantum Dots: WORKPLAN

This is a detailed work plan of the activities to be performed during this KURF program. In the end, it is expected that the student will deliver a detailed report of the activities carried out including a scientific results and soft-skill training.

1. Theoretical Background:

In this part of the KURF program, a comprehensive review will be carried out encompassing the physical properties of InP Quantum Dots, and the computational methodologies used to study them, namely, Force Fields and *ab-initio* calculations.

Activities:

→ *In-P Quantum Dots:* Experimental studies and measured properties, simulation techniques used to perform computational studies, challenges and possible solutions.

→ *Computational methods:* Basic introduction to electronic structure calculations, Density Functional Theory, and physical properties of Quantum Dots.

2. Programming training:

This section describes the programming skills that the project requires to be developed. As a final result, the analysis of data and written scripts will be added in the final scientific report.

Programming languages: Python, Bash, HPC general usage.

3. Computational work:

In this section, the main objective is to perform *ab-initio* calculations for obtaining important quantities such as total energies and electronic structure properties.

Program: CP2K
Cluster: Young

Calculations to be performed:
→ Relaxation of structures
→ Single Point energy calculations
→ Bond energies
→ Alloy energies

4. Results and analysis:

In this section, the analysis of the computed results will be carried out. Different visualization techniques will be used to display and interpret the obtained results.

Programming skills: Python scripting, Python Matplotlib, Python Numpy, Sapphire

Analysis:

→ Convex hull energy dissociation
→ Convex hull alloy energy

→ Radial distribution functions and local environment analysis

5. Scientific report

As a final stage of the project, a scientific report must be delivered and submitted to KURF's central committee. This report will consist of 3 parts:

→ **Introduction:** State-of-the-art research in InP Quantum Dots. Important results and challenges to produce and predict desired properties in these systems.

→ **Results and analysis:** Discussion about the results obtained from the computational simulations. Structure-property relationships with a special focus in energy/electronic properties vs radius diameter and description of local environments (In-P bonds and neighbours).

→ **Conclusions and appendices:** Based on the previous results, general trends can be drawn. Appendices will contain the post-processing scripts used in this KURF's project. Input files of the calculations will be stored in Lorenz's lab GitHub repository.