Polymers: 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 scientific results and soft-skill training.

1. Theoretical Background:

In this part of the KURF program, a comprehensive literature review will be carried out encompassing the definition of a polymer and the computational methodologies used to study them, namely, Force Fields and ab-initio calculations.

Estimated time: 2-3 weeks
Activities:

→ Polymers : What is a polymer and the characteristics of the molecules used to create these polymers (Donors, Acceptors and Bridges).

→ Computational methods: Basic introduction to electronic structure calculations, Density Functional Theory.

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 excited state energies and electronic structure properties.

Estimated time: 4-5 weeks

Program: GFN-xTB/ORCA
Cluster: Young

Calculations to be performed:
→ Relaxation of selected structures (50) to compare the accuracy of different methodologies.
→ Comparison between CCSD(T) and DFT (50) electronic structure properties to gauge the accuracy of the employed DFT approach for the database calculation.

Software-development:
→ Organization of a polymer database with 25.000 unique polymers. This includes to create a Python workflow to print using the .cjson format.

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.

Estimated time: 1-2 Weeks

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

Analysis:
→ Distribution of HOMO-LUMO gaps.
→ Distribution of Dipole moments.
→ Distribution of Polarization Inertia tensor.
→ Clusterization of polymers based on physical properties and fingerprints

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:

Estimated time: 1-2 weeks

→ **Introduction:** State-of-the-art research in polymer physics. 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.