IAC Lehrstuhl für Bioanorganische Chemie | RWTH AACHEN UNIVERSITY

Internship: Machine Learning (ML) based development of regression models for sustainable catalytic polymerization reactions

Who are we?

The Herres-Pawlis group aims at the development of highly efficient lactide polymerization catalysts by exploring the synergy between the chemical workflows and a variety of ML-based algorithms. To date, the Herres-Pawlis group has deduced the 3-D structures of almost 100 catalytically active complexes by single crystal X-ray crystallography. Density Functional Theory (DFT) was further explored for the calculation of electronic and quantum properties of these complexes. Now, the derived principles will be transferred to further complexes.

Task Description:

You will be responsible for the collection of dataset from the lactide polymerization literature and then perform the optimization of the structures using the DFT principles. Then the development of ML models will be accomplished using the modules of the Python programming language. Afterwards, the generated ML models will be used for the calculation of the associated properties essential for the polymerization.

Requirements:

1) Experience in Python programming language or DFT.
2) Interested in working with Machine Learning.
3) Can take up the task to learn the Computational Chemistry tools or Python.
4) Dedicated to solving the problem independently.

Interested Candidates can forward their CV!

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