

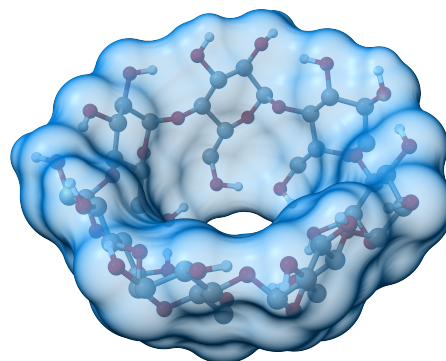
Transfer Learning of Graph Neural Networks for Implicit Solvent Modeling

Background and Motivation

Molecular dynamics (MD) simulations are essential for understanding the dynamical properties of proteins and other molecular systems. While highly accurate, traditional simulations are computationally expensive. Machine learning potentials (MLPs), particularly those based on advanced **Graph Neural Networks (GNNs)**, provide a promising alternative by balancing physical accuracy with computational efficiency.

A major bottleneck is the **explicit solvent simulation**: tracking every water molecule is very costly. **Implicit solvent models** avoid this by representing the solvent as a continuous medium, which keeps key physics while reducing computation.

In this thesis, you will combine **GNNs** with **parameter-efficient transfer learning** (e.g., **LoRA**) to adapt **pre-trained MLPs** to implicit solvent settings. The goal is a method that is accurate, scalable, and efficient for implicit solvent simulation.



Objectives

- Understand modern **GNN architectures** for molecular potentials.
- Apply **LoRA/adapters** to transfer **pre-trained models**.
- Build **implicit solvent representations** in the model.
- Evaluate **accuracy, transfer performance, and runtime efficiency**.

Candidate Profile

We are looking for technically strong Master's students with a keen interest in AI/ML methods and their scientific applications. Preferred skills and interests include:

- Familiarity with probability theory and statistics.
- Interest in dynamical systems, physics, chemistry, or applied mathematics.
- Strong time management and a proactive mindset.

What You Will Gain

- Hands-on coding and experimentation with state-of-the-art AI methods for physics-inspired problems.
- Learn how to collaborate with others in an international research environment.
- Opportunities to contribute to high-quality scientific publications.

Application

If interested, please email linyong.zhang@tum.de with:

- A brief introduction with your background and motivation.
- Your transcript of records.