Professorship of Multiscale Modeling of Fluid Materials
TUM School of Engineering and Design

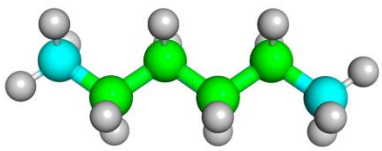
Research Project / Thesis Opportunity

Title
Training Strategies for Coarse-grained Machine Learning Potentials

Project Description
Machine learning potentials (MLPs) are an emerging approach that bridges the gap between quantum-mechanical accuracy and classical molecular dynamics. Coarse-graining, which reduces the system's degrees of freedom, is essential for accessing larger length scales and longer timescales. The application of MLPs to coarse-grained systems has only recently begun, and in this project, we aim to explore and optimise different training strategies.

Project Aims
- Explore different training strategies for coarse-grained machine learning potentials
- Augment data pipelines and machine learning model architecture
- Perform ablation studies to assess model performance

Requirements
- Programming experience: proficiency in Python
- Experience working with molecular data



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Ns = 3

Contact
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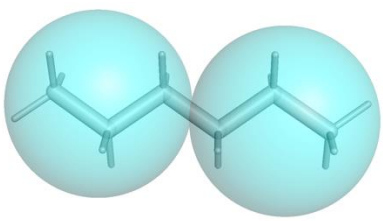

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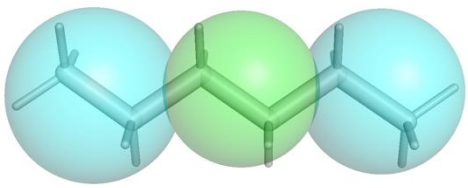

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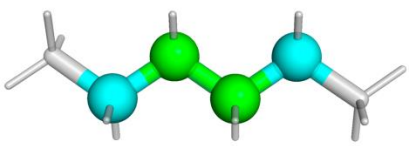

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