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| KIT-Campus Nord | ITES | Postfach 3040 | 76021 Karlsruhe | **Institut für Thermische Energietechnik  und Sicherheit (ITES)**  Leiter/in: Prof. Dr. D. Banuti  Wiss. Betreuung:  Prof. Dr. D. Banuti  Hermann-von-Helmholtz-Platz 1  76344 Eggenstein-Leopoldshafen  Telefon: 0721 6082-3451  E-Mail: secretary@ites.kit.edu  Web: https://ites.kit.edu |
| **Master Thesis**  **Molecular dynamics simulations of  high-pressure fluids  (numerical / theoretical)** |

In the pursuit of more efficiency, operating pressures have increased over the decades in power plants, jet engines, internal combustion engines and organic Rankine cycles. Often, supercritical pressures are reached in these processes, leading to fluid behavior that deviates dramatically from the well-known ideal gases or constant density liquids and still offers some exciting new insights over the last years.

The goal of this thesis is to use molecular dynamics simulations to drive our understanding of supercritical fluid behavior, by studying molecular interactions and group behavior.

The thesis requires

- knowledge in thermodynamics / heat transfer / numerical methods

- ideally experience with numerical simulations

- experience or interest and willingness to learn Python/Jupyter notebooks for data analysis and simulations using the LAMMPS open source molecular dynamics solver.

Specifically, the work will involve

- literature research on supercritical fluid molecular structure

- LAMMPS simulations of fluid behavior under various boundary conditions

- analysis of results

- documentation and dissemination (thesis, presentation, possibly paper) of the work

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