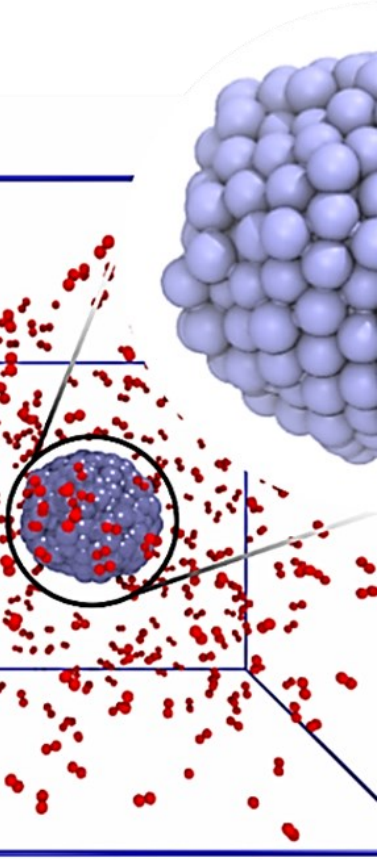
Master-Thesis

Investigation of iron-oxide nanoparticle formation using force-field-based molecular dynamics (MD) simulations

TECHNISCHE UNIVERSITÄT DARMSTADT

RSM Reaktive Strömungen + Messtechnik



Motivation & Background

The project Clean Circles is dedicated to solving global energy problems by using iron as CO2-free, renewable and chemical energy carrier. Electricity from renewables is used to reduce iron oxide (energy storage). Then, the iron is oxidized to release thermal energy for electricity generation at a different place and time (energy release). In the project, scientists and students from different universities work closely on numerous experiments and simulations.

Investigating the underlying mechanisms of iron-oxide nanoparticle formation is crucial yet challenging via an in-situ experimental technique due to the high-temperature environment and fast-evolving kinetics. With increasing computational capabilities, empirical force-field-based molecular dynamics (MD) approaches have emerged as valuable complements to experiments for probing atomic interactions in complex physicochemical systems. In this thesis, the ReaxFF-MD method should be implemented to study the iron-oxide nanoparticle formation mechanism during metal powder combustion.

This work will be closely co-supervised by our partner from U.S. and thesis and presentations have to be given in English. With excellent outcome, it also opens opportunities to present your results at international workshops or conferences.

Tasks

- Review the literature, especially metal power combustion and MD simulations
- Implementation of ReaxFF-MD approach for simulation nanoparticles and their precursors
- Performing simulations with controlled variables and boundary conditions
- Analyzing data and results
- Intermediate and final presentations, writing final theses

Focus areas

Experiment	●○○
Construction	○○○
Modeling	●●●
Data analysis	●●●

Date

22.03.2024

Start from

Flexible, get in touch!

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