Master Thesis (M.Sc.)

Molecular dynamic simulation of ash melting behavior in silica-rich biomass ashes

BACKGROUND AND OBJECTIVE:

Thermochemical conversion is the most common route to produce biogenic silica from silica-rich biomass assortments such as rice husk (RH) and rice straw (RS). This process can contribute to sustainable reduction of greenhouse gas emission in mid and long term perspective. One of the major challenges in this process is high ash melting tendency of RH and particularly RS. In order to mitigate the ash melting during the thermochemical conversion, information about the ash transformation mechanism is vital. A comprehensive research investigation, which was performed at DBFZ [1] showed that advanced spectroscopic and diffractometric techniques are useful tools to characterize crystalline phases of silica-rich ashes. However, the amorphous share of the ashes requires additional tools to be characterized. In this respect, FactSage simulation provided useful information about phase composition of untreated and chemically pretreated RH and RS ashes [1]. Furthermore, molecular dynamic simulation (MD) can be used to simulate the melting behavior of biomass ashes [2, 3]. Thus, with the aim of the present master thesis will be used to simulate the ash melting behavior of the crystalline and amorphous phases and to validate the model with available spectroscopic and diffractometric data of the ashes.

YOUR TASKS:

- Evaluation of the state of knowledge for molecular dynamic simulation of biomass ash behavior.
- Development of appropriate atomic structural information and potentials for each particular ash phase.
- Evaluation of crystallographic information files (CSF) using open source software packages e.g. VESTA [4].
- Molecular dynamic simulation of different amorphous and crystalline phases using LAMMPS [5].

YOUR PROFILE:

- Academic degree in inorganic chemistry, material sciences, chemical engineering or comparable
- Experience in computational chemistry, especially in MD is beneficial
- Interested in crystallographic, numerical data evaluation and thermochemical conversion
- Good English language skills

WE OFFER:

- Advanced computational and research facilities
- A good introduction to the topic as well as competent and motivated support in the processing of the tasks
- A family-friendly, modern working environment in a collegial working atmosphere and good public transport connections

The project shall be carried out in English. Furthermore, the work can be prepared remotely.

POSSIBLE STARTING DATE:

January 2022

DURATION:

At least 2 months. It can also be extended for 6 additional months for a master thesis

BEARBEITUNGSORT:

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BEWERBUNGSUNTERLAGEN:

Please provide your application including letter of motivation and current enrollment certificate (only 1 attachment, preferably as pdf, max. 5 MB). E-mail: bewerbung@dbfz.de

For an encrypted transmission of your you can use the upload platform Cryptshare: www.dbfz.de/stellen

REFERENCES:

[1] Beidaghy Dizaji H, Zeng T, Hölzig H, Bauer J, Klöß G, Enke D. Ash transformation mechanism during combustion of rice husk and rice straw. Fuel;307:121768; 2022. https://doi.org/10.1016/j.fuel.2021.121768.
[2] Ma, C., Skoglund, N., Carlborg, M., & Broström, M. (2021). Structures and diffusion motions of K and Ca in biomass ash slags from molecular dynamics simulations. Fuel, 302, 121072.
[3] Ma, C., Skoglund, N., Carlborg, M., & Broström, M. (2020). Viscosity of molten CaOK2OSiO2 woody biomass ash slags in relation to structural characteristics from molecular dynamics simulation. Chemical Engineering Science, 215, 115464.
[4] Momma K, Izumi F. VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data. J Appl Crystallogr 2011;44(6):1272–6.
[5] https://www.lammps.org/.