We currently have an opening for a

Postdoc (m/f/d)
(TV-L 13, full time, 2 years)

DESIGNING AQUEOUS DEEP EUTECTIC MIXTURES BY DATA-INTEGRATED SIMULATION

The Cluster of Excellence "Data-Integrated Simulation Science" (EXC 2075) is an interdisciplinary research center with more than 200 scientists performing research towards a common goal: We target a new class of modeling and computational methods based on available data from various sources, in order to take the usability, precision and reliability of simulations to a new level.

THE PROJECT

The goal of the project "**Designing aqueous deep eutectic mixtures by data-integrated simulation**" is to develop and apply a design strategy for deep eutectic solvents by combining molecular dynamics simulations and machine learning strategies. Deep eutectic solvents (DES) are promising solvents in biocatalysis, because they are designable, renewable, biodegradable, and cheap. Thus, they are considered as an alternative to organic solvents for enzyme-catalyzed reactions that involve hydrophobic substrates. The thermophysical properties of aqueous DES mixtures such as density, melting point, viscosity, substrate solubility, and thermodynamic activity of water can be designed by varying the components, their mole fraction, and the temperature. Thus, a very large design space is available. Molecular dynamics simulations provide an atomistic understanding of thermodynamic and transport properties, which is essential to guide the design of DESs. To reduce the computational expense of screening the design space, a combination of MD simulations with machine learning methods will be applied.

YOUR TASKS

- Follow best practices in sustainable software development and apply and further develop a scalable workflow environment to perform large-scale simulations on a HPC infrastructure
- Follow the F.A.I.R. data principles and systematically compare thermophysical properties obtained from simulations to published experimental data by using ThermoML
- Use the simulation results for machine learning and for improving the force fields of the compounds in the complex mixtures.
- Design novel deep eutectic solvents and validate the predictions in collaboration with our experimental project partners
- Contribute to the teaching activities of the host group

WE ARE LOOKING FOR

We seek strong applicants with a Doctorate in Chemistry, Chemical Engineering, Biotechnology, Physics, or a closely related field ideally with a specific focus on molecular simulation and experience in machine learning techniques. We value diversity and want to specifically encourage applications from underrepresented groups. Successful candidates should be curiosity-driven, ambitious, creative, and passionate about interdisciplinary research in the area of simulation and data sciences. Strong team working and critical thinking skills,

aptitude for independent and creative work, as well as fluent English written and presentation skills are essential.

The position is fully funded (100%) and is available to applicants of any nationality. You will contribute to the leadership of ongoing projects, will have the opportunity to advise undergraduate and graduate students, and contribute to the teaching activities of the group.

If you are highly motivated and capable of addressing and solving scientifically difficult problems and if you are interested in doing research in an internationally oriented and highly successful team, you should send your application to jobs@simtech.uni-stuttgart.de. Please submit your complete application by e-mail with one pdf attachment comprising a cover letter, academic CV, research statement, a full publication list, names and contact addresses of two referees, as well as academic certificates and transcript of records.

If you have any questions regarding this application, please contact Prof. Jürgen Pleiss (Juergen.Pleiss@itb.uni-stuttgart.de).

We cannot reimburse any costs arising from the performance of job interviews.

The University of Stuttgart has been awarded "family-friendly employer". Flexible working hours, regular child care services, and family-networks allow for a better combination of professional and family life. The University of Stuttgart also offers a range of services to enhance social equity (https://www.uni-stuttgart.de/en/university/profile/equality-diversity/). Additionally, a dual career program is in place to offer assistance to partners of those moving to Stuttgart. For more information, please visit https://www.uni-stuttgart.de/universitaet/arbeitgeber/dualcareer/

The University of Stuttgart is an equal opportunity employer. Applications from women are strongly encouraged. Severely challenged persons will be given preference in case of equal qualifications.

Information on the collection of personal data in accordance with Article 13 of the GDPR can be found via the following link: https://www.uni-stuttgart.de/en/privacy-notice/job-application/