Stellentyp: Masterarbeit, Projektarbeit, Studienarbeit

Ausschreibungsdatum: ab 26.11.2018

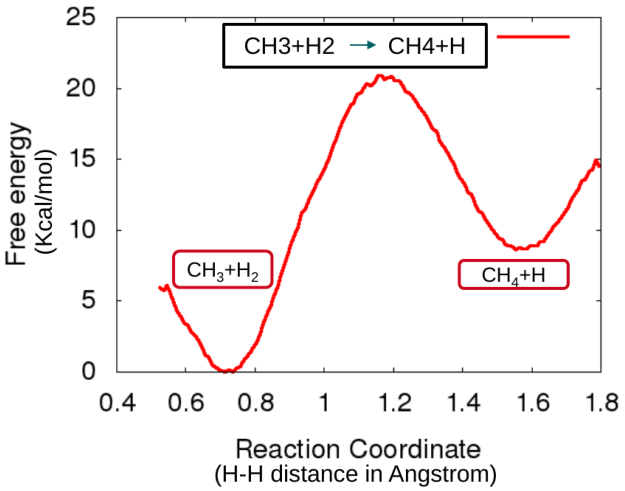
Determining Reaction Rate from Free Energy Calculation

Our Profile:

In the working group "Model based fuel design" at the Chair of Technical Thermodynamics molecular dynamics and quantum mechanics is used to study reaction kinetics. Through the study of reaction kinetics we try to make combustion efficient, so that environmental consequences can be minimized.

Your Task:

Chemical reactions with slower kinetics are not pragmatic to simulate with molecular dynamics as it takes immense computational time to simulate the reactions. Statistical sampling method is used to capture the reaction through pre-defined reaction coordinate. Such methods will be validated against molecular dynamics and transition theory from quantum mechanics. You will work with LAMMPS software.



Our Offer:

Do your project under supervision of a motivated team. You will get an insight into scientific working methods and deepen your knowledge in programming, molecular dynamics and combustion chemistry.

Your Profile:

Ideally, you are

- having interest in molecular thermodynamics
- enthusiastic to learn new software
- comfortable with programming language

Feel free to contact me at:

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