Improved Hydrogen bond modeling for the
HyDRA benchmark challenge

Our profile:

The research group Molecular Systems Engineering (MSE) of the Institute of Technical Thermodynamics (LTT) headed by Prof. Leonhard focuses on the design of molecular systems in energy and chemical engineering. We focus on predicting accurate thermochemical data, namely, enthalpy, entropy, free energy, specific heat capacity etc. using quantum chemical calculations. In addition to this, we also predict accurate spectroscopic data in close collaboration with experimental groups at LTT. Since 2017, MSE has taken part in international benchmark challenges and our methods performed among the most accurate ones.

Background:

MSE took part in a blind challenge organized by the Chemistry department at the University of Göttingen. We submitted the water stretch frequency data for four 1:1 organic-water complexes. While the submitted data lies in the expected error range, we can further increase the accuracy by tinkering with the parameters for the calculations. In addition to this, the computer experiments are conducted using the commercial softwares in the RWTH high performance computing centre. The data generated will be pushed for a publication from Prof Leonhard's group.

Your task:

- Perform quantum mechanic calculation using the software Gaussian for finding the water stretche frequency in the 1:1 organic-water complexes.
- Create an automation framework in atomic simulation environment to run the calculations.
- Discussion and validation of the results: In the project, we have experimental frequencies for validation.

Your profile:

- Students with Chemistry / Physics / Mechanical Engineering / CES Energietechnik / Verfahrenstechnik or similar backgrounds.
- Programming skills, especially with Python, are necessary.
- Good knowledge of / interest in quantum mechanical methods and chemical reactions.
- Out of the box thinking and a careful and independent way of working with good command of English language.

What you can get from the project:

You will work on a very innovative topic and will attain a commendable level of insight into the field of spectroscopy and quantum chemistry. Skills and knowledge in the field of quantum mechanical simulations, automation and working with python will be enhanced. The enthusiastic, motivated and an innovative team of MSE is looking forward to meet you. If you are interested in the topic, please write to Narasimhan Viswanathan by e-mail (narasimhan.viswanathan@ltt.rwth-aachen.de) with CV and transcripts.