We are one of the youngest universities in Germany and think in terms of possibilities, not limitations. In the heart of the Ruhr Area, we develop ideas of the future at our 11 faculties. We are strong in research and teaching, in living diversity, as well as in supporting potential. We are highly committed to an educational equality that has earned this name.

The **University of Duisburg-Essen** at the **Faculty of Physics**, Theoretical Physics, Duisburg Campus invites applications for the position of a

Scientific Researcher (f/m/d)
(Payment according to Grade E 13 TV-L)

Main research topics and duties:

Participation in the research project **Development of novel microsolvation models with coupling to local grand-canonical ensembles**.

The simulation of the effect of solvation on physico-chemical processes with *ab initio* calculations usually relies on implicit solvation models, where the solvent degrees of freedom are not treated explicitly. Such a partitioning in an explicitly described system and a surrounding solvent bath requires the assumption of weak interaction, which is not always valid. Hybrid models, where part of the solvent is described explicitly, improve the accuracy. However, there is no consensus about how to construct such models systematically.
It is the goal of this position to develop such hybrid models, where the explicitly treated solvent molecules are coupled to local grand-canonical ensembles (characterized by a temperature and a chemical potential). Starting from a simple hard-sphere solvent, more refined models will be developed that allow for the hierarchical construction of microsolvated complexes. Molecular dynamics simulations will aid the parameterization of the local grand-canonical ensembles. For strongly coupled solvents, the combination with different solvation models will be investigated.

Participation in the preparation of courses and teaching duties are also expected.
As part of this graduate position, the successful applicant is offered ample opportunity for further scientific training (culminating in a PhD).
The position is supported by the RESOLV cluster of excellence (Ruhr Explores Solvation, www.solvation.com). Participation in the integrated RESOLV graduate school is required.

Required qualifications:
Completed university studies in physics or chemistry of at least 8 semesters. A top-level thesis
(< 1.5 in the German system) and top-level graded courses are required. A very good command of written and spoken English is essential.
In addition, knowledge of electronic-structure theory and statistical physics, first experience in the application of DFT programs (Q-Chem, Orca or similar), and programming experience in common languages (C++, Fortran, Python) are desired.

We offer:

- a varied, versatile range of tasks
- further education offers Firmenticket
- discounted company ticket for public transport
- opportunity to participate in sports and health programs (university sports)

Expected start of position: as soon as possible

Contract period: 3 Years

Working time: 75% of a full time employment

Application deadline: 03.09.2021

The University of Duisburg-Essen aims to increase the diversity of its members (see http://www.uni-due.de/diversity). It also aims to increase the number of women among its academic staff and therefore encourages women with pertinent qualifications to apply.

Women with equal qualifications will be preferred in accordance with state equality laws. Applications of qualified disabled persons in the legal sense of § 2 para. 3 SGB IX are also welcome.

Please submit your application (motivation letter, CV, diplomas, transcript of modules taken with grades, a letter of recommendation) quoting reference **494-21** to Dr. Christopher J. Stein, Universität Duisburg-Essen, Fakultät für Physik, Lotharstr. 1, 47048 Duisburg, or, preferably in a single pdf-file, to christopher.stein@uni-due.de.

Information on the faculty and the advertised vacancy is available at:
https://www.uni-due.de/physik/index_en.php
https://www.uni-due.de/en/index.php
www.uni-due.de