The VGSCO currently announces a PhD position in the area of

Optimization Techniques in Data Science, with Applications to Molecular Chemistry
(University of Vienna, Supervisor: Arnold Neumaier)

For molecular dynamics simulations of complex molecules, good potential energy surfaces must be available. In principle, these can be computed by ab initio quantum chemistry techniques, but these are extremely time-consuming. Therefore, one generally uses empirical potential energy surfaces fitted to ab initio (or experimental) data using various optimization techniques.

The main topic of this thesis project is the construction of mathematical models for potential energy surfaces of complex molecules, and the development and analysis of algorithms facilitating such a construction.

In recent years, machine learning tools have been successfully used to construct such empirical potentials defined in terms of neural networks. The project aims to utilize these and more traditional optimization techniques to construct a family of potentials that accounts for all ab initio data from the literature about molecules composed of hydrogen and oxygen atoms only.

The candidates are expected to have a solid theoretical and computational background in optimization, numerical analysis, linear algebra, and considerable experience with implementation of algorithms. Basic knowledge of molecular modeling and quantum chemistry are an advantage.

The advertised position is associated with the Faculty of Mathematics of the **University of Vienna** in the Research Group Computational Mathematics of **Prof. Dr. Arnold Neumaier**. The successful candidate will become a member of the **Vienna Graduate School on Computational Optimization**. An enrolment in the **Vienna School of Mathematics** is also envisaged. The duration of the employment is of 3 years with possibility of extension. The extent of employment is 30 hours per week. The annual gross salary is approximately 31,000 €. The planned start of the position is autumn 2020.

Application Requirements and Procedure

The candidates must have a master degree (or equivalent) in *Mathematics, Computer Science, Data Science* or *Statistics* at the moment the PhD position starts. The application documents should contain a letter of motivation; the scientific CV with publication list, if available; higher education certificates/diplomas; the diploma/master thesis and letter(s) of recommendation. Applications have to be submitted at: **vgsco.univie.ac.at/positions/application**. The deadline for applications is **August 31, 2020.**