Summer Student Project Theoretical Chemistry (2024 Köster Group)

Elucidation of Reaction Mechanism

The elucidation of reaction mechanism is a fundamental prerequisite towards a rational approach to Chemistry. In this project reaction mechanisms of intramolecular Diels-Alder cyclization will be investigated with the hierarchical transition state finder of deMon2k (see www.demon-software.com). The aim of the study is to rationalize the unusual product distributions based on quantum chemical calculations. To this end, reactant and product structures will be optimized from parallel-tempering Born-Oppenheimer molecular dynamics trajectories. These structures are then used in a hierarchical transition state search to find activated complexes from which intrinsic reaction coordinates are calculated.

The successful applicant will be provided with a workspace in the Theoretical Chemistry group of Dr. Köster and will have access to all local compute facilities. After a basic introduction into quantum chemical calculations, the student will learn how to optimize molecular structures with first-principles density functional theory methods. For the search of non-intuitive transition states an introduction into the use of the hierarchical transition state finder will be given. Prior knowledge of quantum chemistry is not mandatory.