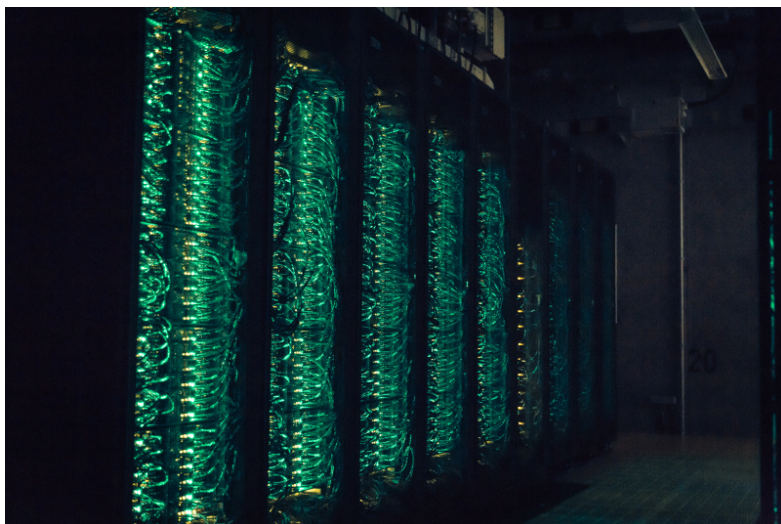


# Functionalization of Hydrocarbons Trough Novel HAT-Agents



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Project Term  
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Project Areas  
Molecular Chemistry

Software  
GAUSSIAN

Additional Software  
Avogadro, Chemcraft

Institute  
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## Introduction

Alkanes are attractive feedstock chemicals due to their natural occurrence and they offer access to a wide variety of substrates by C-H functionalization. This can be achieved by highly reactive species like carbenes, radicals, carbocations etc. However, selective functionalizations are still rather challenging. On the basis of several heterocyclic compounds (2(3H)-thiazolone, 2(3H)-thiazolthione, 2-imidazolone, 2-imidazolthione) we want to generate highly reactive radical cations, which subsequently undergo selective HAT from unactivated C(sp<sup>3</sup>)-H-bonds of hydrocarbons to generate carbon centered radicals. These radicals will afterwards be trapped by electrophilic group transfer agents (tosylcyanide, tosylazide, etc.) to form functionalized hydrocarbons.

## Methods

We are using Gaussian16 for modeling organic compounds, compare their ground state energy and calculate binding dissociation energies (BDE) through a homodesmotic equation set. For our needs to compare experimental data with theory we need to compute our structures on a high level of theory. As basis for geometry optimization and energy calculation serve Double-Hybrid-Methods such as B2PLYP/6-311G(d,p). In each of our investigated systems it is very important to know BDEs in order to find suitable systems which exhibit BDEs higher then 100 kcal/mol to facilitate HAT from unactivated C(sp<sup>3</sup>)-H-bonds.

## Results

In the first period we were able to compute small closed- and open-shell structures to understand the influence of their substitution pattern on their stability, electrophilicity and BDE. Ongoing investigations are about the dynamics of HAT on the basis of a curve crossing model and the development of new systems to achieve selective HAT.

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