

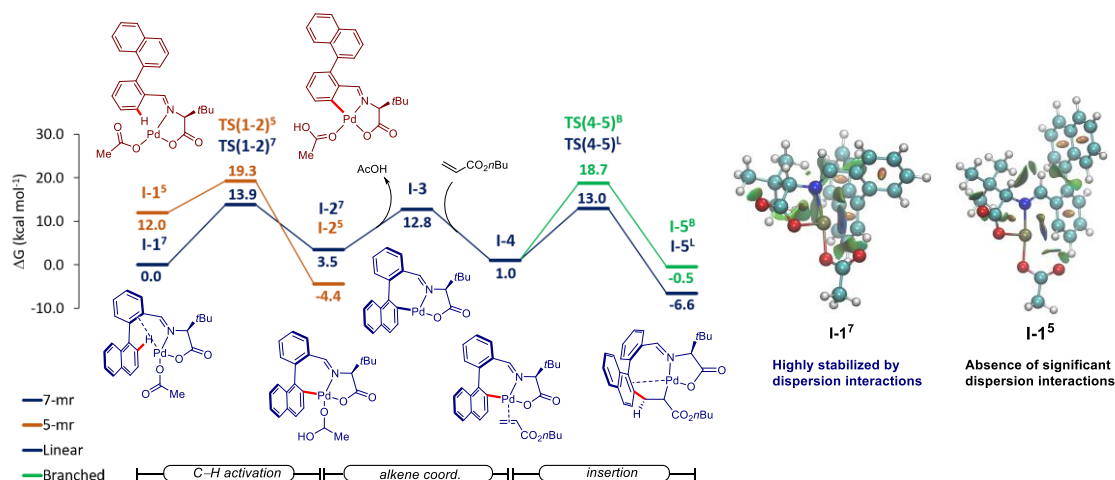
## PhD project at the University of Göttingen

Principal Investigator: Prof. Dr. Lutz Ackermann

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PhD Project Title: Modelization and mechanistic studies on asymmetric C–H activation

PhD Project description: The interplay of computational with experimental chemistry is key to unravel mechanistic insight. Recently, data analysis to enable the prediction of a reaction outcome and machine learning based reaction optimization has gained considerable attention. To this end, the Ackermann group performed detailed experimental mechanistic studies in combination with computational models.<sup>1</sup> In this regard, the forces behind the preferred selectivity in enantioselective pallada-electrocatalyzed C–H activation by transient directing groups to access chemically relevant helicenes motifs have been narrowed down:<sup>2</sup>



Description of the work: The project will be highly collaborative and aim to study fundamentally new C–H activation concepts with a topical focus on asymmetric transformations. The work will be mainly related to computational chemistry (DFT, ML...), although experimental work will be possible if the candidate is interested. ESR3 will: 1) simulate chiral ligands prompt to induce chirality in direct C–H transformations; 2) re-optimize ligands in terms of enantiomeric excess and yield following experimental results; 3) identify key parameters controlling asymmetric C–H activation; 4) design a library of chiral ligands for asymmetric C–H activation for the generation of predictive models by ML to predict novel and highly efficient chiral ligands.

Relevant skills that will be considered are:

- Interest in catalysis
- Existing knowledge and experience in computational chemistry is required
- Experience and theoretical background in C–H activation are of advantage
- Good level of English proficiency (understood, spoken and written)
- Skills in scientific writing (reports, papers, etc.)
- Team spirit and collaborative predisposition

Planned secondments: Secondments Syngenta (M15-M17): Adaptation and upscaling of the modeled templates; use of high throughput experimentation; AstraZeneca (M33-35): late-stage functionalization of bio-relevant scaffolds.

<sup>1</sup> a) M. Stangier, A. M. Messinis, J. C. A. Oliveira, H. Yu, L. Ackermann, *Nature Communications* **2021**, 12, 4736; b) T. H. Meyer, J. C. A. Oliveira, D. Ghorai, L. Ackermann, *Angew. Chem. Int. Ed.* **2020**, 59, 10955-10960.

<sup>2</sup> U. Dhawa, C. Tian, T. Wdowik, J. C. A. Oliveira, J. Hao, L. Ackermann, *Angew. Chem. Int. Ed.* **2020**, 59, 13451-13457.