

Vortragsankündigung

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Es spricht: **Prof. Dr. R. Tom Baker**, Canada Research
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Ort: **TU Berlin**
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Thema: **Mechanistic Studies of Metal Complex-
Catalyzed Ammonia-Borane
Dehydrogenation: A Promising Material for
Chemical Hydrogen Storage**

Abstract: With both protic N-H and hydridic B-H bonds as well as three hydrogen atoms per main group element, ammonia-borane (AB, H_3NBH_3) is a promising material for chemical hydrogen storage applications. Detailed studies of the dehydro-oligomerization of AB has revealed a wealth of reaction products and reaction pathways depending on reaction media and conditions, additives and catalysts. Our previous studies on acid-catalyzed thermolysis served to bolster our understanding of intermolecular AB dehydrogenation in the solid state, in ethereal solutions and in ionic liquids. Previous reports of metal-catalyzed dehydrogenation of AB reported formation of insoluble aminoborane cyclic pentamer, $(\text{H}_2\text{NBH}_2)_5$, or soluble iminoborane cyclic trimer (borazine, $\text{B}_3\text{N}_3\text{H}_6$) and corresponding B-N linked borazines (polyborazylene). Through detailed *in situ* NMR studies of AB dehydrogenation using a variety of catalyst precursors we have identified a key reaction intermediate proposed to arise by trapping of reactive aminoborane monomer, (H_2NBH_2) , by AB. This intermediate is converted directly into borazine and polyborazylene, thus yielding > 2 equiv. of H_2 per AB. Competing formation of aminoborane pentamer (and only 1 equiv. of H_2) is proposed to arise from retention of aminoborane monomer in the metal's coordination sphere followed by a dehydrogenative metallacycle growth pathway. A new family of chelating diamine bis(phosphine) iron catalysts is proposed to dehydrogenate amine-boranes via a Noyori-type heterolytic activation mechanism. Finally, remaining technical barriers to commercialization of amine-borane fuels are described.

Organisator: **Prof. Dr. M. Driß (TUB)**

Gäste sind herzlich willkommen!

Prof. Dr. Matthias Driß

Sprecher des Exzellenz-Clusters UniCat