**From biological to heterogeneous catalysis: Spectroscopic studies of dinitrogen reduction**

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The conversion of dinitrogen (N2) to ammonia (NH3) is of fundamental biological and economic importance. The catalytic conversion is achieved either industrially, using heterogeneous catalysts or biologically, by the nitrogenase enzyme. However, in both cases, the mechanistic details of the process are not fully understood. In order to design advanced catalysts that will be essential for a sustainable energy economy, an in-depth understanding of both the biological and chemical mechanisms is required. The focus of my research group goal is on the development of advanced spectroscopic tools, which allow for a detailed description of the atomic level processes in the both the biological and the heterogeneous systems. Specifically, a range of X-ray-based spectroscopic methods is utilized as a unique probe of transition metal active sites in complex media. High-resolution X-ray absorption spectroscopy (HERFD XAS), X-ray emission spectroscopy (XES), X-ray magnetic circular dichroism (XMCD), and scanning transmission X-ray microscopy (STXM) are utilized, and their chemical information content fully developed using model systems, before applying these methods to the real catalysts. These experiments are correlated to advanced quantum chemical calculations to obtain a detailed picture of the electronic structure of the catalytic systems. Recent advances in our understanding of the FeMo and FeV cofactors of nitrogenase and iron-based ammonia synthesis (and decomposition) catalysts will be presented.