X-RAY SPECTROSCOPIC STUDIES OF NITROGENASE AND HYDROGENASE ACTIVE SITES

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The efficient storage and release of energy in chemical bonds is a fundamental goal of molecular energy research. It is here that Nature provides an ideal paradigm in that earth abundant metals are utilized to enable bond formation and cleavage. Recent research in our laboratory has focused on understanding the fundamental chemistry of dintritrogen reduction and hydrogen production by the nitrogenase and hydrogenase families of enzymes, respectively. The development and application of advanced X-ray spectroscopic methods to detect the presence of single ligated atoms (e.g. carbide or hydride) will be highlighted. The ability to use valence-to-core X-ray emission spectroscopy as a measure of small molecule activation, as well as two-dimensional X-ray spectroscopic approaches for enhanced selectivity, will be discussed.[1,2] Recent advances in our understanding of the electronic structure of the nitrogenase and hydrogenase actives sites will be emphasized.[2-9]

(1) Hall, E. R.; Pollock, C. J.; Bendix, J.; Collins, T. J.; Glatzel, P.; DeBeer, S. *Journal of the American Chemical Society* **2014**, *136*, 10076.
(2) Pollock, C. J.; Grubel, K.; Holland, P. L.; DeBeer, S. *Journal of the American Chemical Society* **2013**, *135*, 11803.
(3) Bjornsson, R.; Lima, F. A.; Spatzal, T.; Weyhermueller, T.; Glatzel, P.; Bill, E.; Einsle, O.; Neese, F.; DeBeer, S. *Chemical Science* **2014**, *5*, 3096.
(4) Bjornsson, R.; Neese, F.; Schrock, R. R.; Einsle, O.; DeBeer, S. *Journal of Biological Inorganic Chemistry* **2015**, *20*, 447.
(5) Lancaster, K. M.; Hu, Y.; Bergmann, U.; Ribbe, M. W.; DeBeer, S. *Journal of the American Chemical Society* **2013**, *135*, 610.
(6) Lancaster, K. M.; Roemelt, M.; Ettenhuber, P.; Hu, Y.; Ribbe, M. W.; Neese, F.; Bergmann, U.; DeBeer, S. *Science* **2011**, *334*, 974.
(7) Pollock, C. J.; DeBeer, S. *Accounts of Chemical Research* **2015,** *48*, 2967.
(8) Rees, J. A.; Bjornsson, R.; Schlesier, J.; Sippel, D.; Einsle, O.; DeBeer, S. *Angewandte Chemie International Edition* **2015**, *54*, 13249.
(9) Hugenbruch, S.; Shafaat, H. S.; Kramer, T.; Delgado-Jaime, M. U.; Weber, K.; Neese, F.; Lubitz, W.; DeBeer, S., *in press.*