

## UniSysCat - Colloquium

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Start Time: Wednesday, July 5, 2023 05:15 pm

End Time: Wednesday, July 5, 2023 06:30 pm

C 264  
or via Zoom

### Hydride and Hydroxide Intermediates in the Catalytic Turnover of Gas-processing Metalloenzymes

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Gas-processing metalloenzymes (GPMs) catalyse challenging reactions exploiting abundant transition metal ions like iron, nickel, or molybdenum. Understanding the structure and molecular mechanism of GPMs inspires the design of synthetic catalysts for H<sub>2</sub> production, N<sub>2</sub> fixation, and the removal of CO<sub>2</sub> from the atmosphere.

Based on insight from structural biology and *in situ* vibrational spectroscopy<sup>(1)</sup>, I will discuss GPMs like hydrogenase<sup>(2)</sup> and nitrogenase<sup>(3)</sup>. Both enzymes bind specialised iron-sulphur clusters that catalyse proton-coupled electron transfer (PCET) processes. Second and outer coordination sphere effects critically promote metal-hydride species that are key to H<sub>2</sub> production with zero electric overpotential and N<sub>2</sub> fixation under ambient conditions<sup>(4)</sup>. Similar concepts help understanding the enzymatic conversion of CO<sub>2</sub> by carbonic anhydrase that exploits metal-hydroxide species in catalysis<sup>(5)</sup>.

Beyond a microscopic understanding of enzymatic turnover, vibrational spectroscopy on [FeFe]- and [NiFe]-hydrogenase complexes allows demonstrating catalytic coupling with CO<sub>2</sub> reduction<sup>(6)</sup>, O<sub>2</sub> reduction<sup>(7)</sup>, and electron bifurcation<sup>(8)</sup>.

References

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3. M. Rohde, K. Laun, I. Zebger, S. T. Stripp, O. Einsle, *Sci Adv.* **7**, eabg4474 (2021).
4. S. T. Stripp et al., *Chem Rev.* **122**, 11900–11973 (2022).
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6. H. M. Dietrich et al., *Nature.* **607**, 823–830 (2022).
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8. A. Katsyv et al., *J Am Chem Soc.* **145**, 5696–5709 (2023).

Prof. Dr. Maria-Andrea Mroginski

Organizer