

Christian Reece

The Rowland Institute at Harvard, Harvard University/USA

Tuesday, 13th September 2022, 16:00 s.t.

TU Wien, Institut für Angewandte Physik, E134
1040 Wien, Wiedner Hauptstraße 8-10
Yellow Tower „B“, 5th floor, SEM.R. DB gelb 05 B

The seminar will be also held as a Zoom Meeting

<https://tuwien.zoom.us/j/97138339991?pwd=U0NHVINMTU5Xd1dMOG0vVkp2MjlrZz09>



Developing New Paradigms for Applied Catalytic Surface Science

Catalytic surface science was developed as a method of “simplifying” the problem of heterogenous catalysis by determining kinetics and mechanisms on compositionally well-defined single-crystal metal surfaces.¹ While fundamental studies are vital to our understanding of catalytic processes, transferring this knowledge to “real-world” catalytic systems is extremely difficult. In an attempt to bridge this (so-called) gap, we are developing instrumentation and methodologies to probe kinetic and mechanistic information with the same resolution as surface science while using “real-world” catalytic materials. We have developed a number of home-built transient packed bed reactors in order to study “real-world” catalytic materials/systems. Using CO oxidation over a Pd catalyst as a test reaction we are able to recreate complex catalytic behaviour witnessed in a UHV molecular beam system² in a packed bed reactor at 108 times higher pressure. Further, we are able to use time-resolved simulations of our transient experiments to demonstrate continuity between the kinetics coefficients measured using molecular beams² and those measured on our materials under “real-world” conditions.

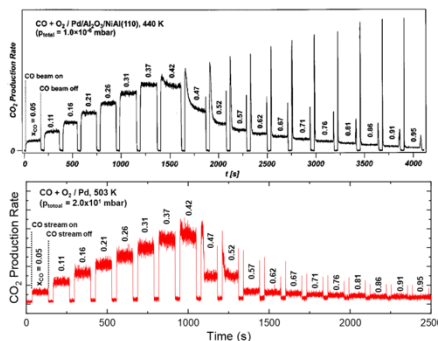


Figure 1. A) A CO oxidation molecular beam experiment performed on Pd/Al₂O₃ model system in UHV. An O₂ beam is fired at the catalyst surface, with a flagged CO beam periodically introduced at varying X_{CO} values.² B) A replicate “pseudo-molecular beam” experiment performed in a packed bed flow reactor atmospheric pressure. The same general trends are identified across 10⁷ times pressure difference. $X_{CO} = (p_{CO}) / (p_{CO} + p_{O_2})$, $p_{total} = (p_{CO} + p_{O_2})$

(1) Reece, C.; Madix, R. J. *ACS Catal.* **2021**, *11* (5), 3048

(2) Libuda, J. et al., *J. Chem. Phys.* **2001**, *114*, 4669

All interested colleagues are welcome to this seminar lecture
(45 min. presentation followed by discussion).

Friedrich Aumayr
(LVA-Leiter)

Gareth Parkinson
(Seminar Chair)