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| הפקולטה להנדסה כימית  ע"ש וולפסון |  |  |
| The Wolfson Department of Chemical Engineering |  |  |

**Wolfson Department of Chemical Engineering Seminar**

**Wednesday, November 24th, 2021 at 13:30**

**Lecture hall #6**

**Formation and Deactivation of Active Sites on Catalyst Surfaces:   
Insights from In Situ Spectroscopy**

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Many catalytic processes suffer from deactivation of the catalyst, during which active sites are destroyed or become inaccessible, whereas other catalytic processes are characterized by induction periods of considerable duration, during which the catalytically active surface species are formed. Several examples of such catalyst behavior will be analyzed in this presentation. Infrared and UV-vis spectroscopy and other analytical methods are applied in situ to follow the surface chemistry. The overarching research objective is to first understand the dynamics of the chemistry on the catalyst surface and, subsequently, use this knowledge to devise strategies to mitigate deactivation, or to accelerate or steer formation of the active sites.

The first two examples focus on catalysis by solid acids, which plays a central role in the conversion of petroleum- and biomass-derived feedstocks to chemicals and fuels. The skeletal isomerization of alkanes on zeolite catalysts is a classic case of deactivation by deposition of carbonaceous matter on the surface. We identify the molecular precursors of these deposits and their charge status by spectroscopy and are able to relate their formation to trace compounds in the feed. In the second example, the conversion of methanol to olefins, long-lived organic surface moieties are actually desired, since they are believed to be part of the catalytically active site (“hydrocarbon pool mechanism”). By using spectroscopic correlations, we can track key surface species and contrast them to published catalytic cycles. The third example is the activation of the Phillips Cr(VI)/SiO2 catalyst for polyethylene manufacture, which has been a mystery since the catalyst’s discovery in 1951. Spectroscopic data are one important piece in solving the puzzle of the active chromium site.