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Limits of Langmuir

Wednesday, 6 December 2017 11:00 (30 minutes)

Langmuir was awarded the Nobel prize in 1932 for his contribution to surface chemistry, a field of utmost importance technically seeing that over 70% of all chemicals are produced in a surface-catalysed reaction. He proposed a bold theory on the adsorption of molecules at surfaces, on which basis the rate of heterogeneously catalysed reactions are typically described. The fundamental assumptions underlying the Langmuir theory include inter alia neglecting adsorbate-adsorbate interactions and single type of surface (site). These conditions are not necessarily fulfilled when dealing with catalysis by metals, especially when dealing with reactions at industrial conditions (high pressure) catalysed by nano-sized metal crystallites.

Theoretical chemistry can give detailed insight in surface chemistry. In particular, the conditions at which adsorbate-adsorbate interactions become important and their consequences can nowadays be easily explored using DFT. In this talk, the adsorbate-adsorbate interactions of species adsorbed on Fe(100) involved in the methanation, and O/OH co-adsorption on Pt(111) and Pt(100)-surfaces will be discussed.

HPC content

Not provided

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