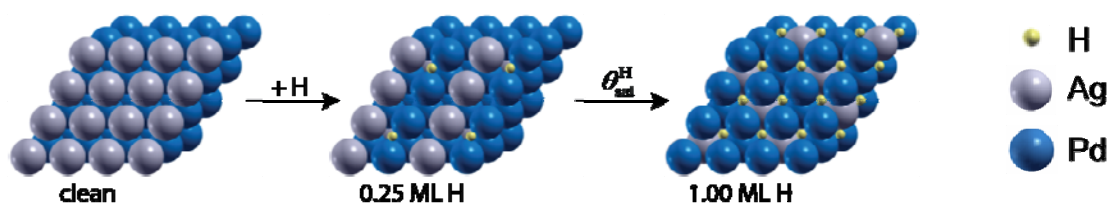


Adsorbate-induced segregation in a PdAg membrane model system

Palladium-silver (PdAg) alloys are suitable candidates for hydrogen separation technologies due to their high selectivity and permeability towards hydrogen. Poisoning effects due to CO and other molecules are well-known, whereas segregation effects of a reactive environment on the (surface) structure and composition of such membranes have been less emphasized. This work employs advanced calculations of the electron structure of PdAg crystals to provide a better understanding of how the adsorption of H₂, CO or O₂ on the surface is affected by the distribution between Pd and Ag in the topmost atomic layer and vice versa, using computational facilities provided by NOTUR. We find that the PdAg membrane surface is Ag rich in the absence of adsorbates. Pd atoms are pulled to the surface upon adsorption of O, H and CO, making the Pd₃Ag(111) surface Pd-dominated at the corresponding saturation coverages. The research is carried out by the Dept. of Chemical Engineering, NTNU, in collaboration with the Dept. of Chemical and Biological Engineering at the University of Wisconsin-Madison, USA.



I-H. Svenum, J. A. Herron, M. Mavrikakis, H. J. Vervik, Adsorbate-induced segregation in a PdAg membrane model system: Pd₃Ag(111), *Catal. Today* 193 (2012) 111-119.