The CO-induced surface reconstruction on Co(11-20)– a combined theoretical and experimental investigation

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The surface dynamics of a model Fischer-Tropsch catalyst upon exposure to CO has been investigated with a combination of experimental and theoretical methods. The surface of Co(11-20) is known to undergo a CO-induced (3x1) surface reconstruction [1,2], involving the anisotropic migration of Co [2] initiating from the step edges, and was therefore chosen as the model surface.

The restructuring was studied with low energy electron diffraction (LEED), scanning tunnelling microscopy (STM), high-resolution photoelectron spectroscopy (HRPES, MATLINE beamline, ASTRID2, Aarhus University), temperature programmed desorption (TPD) and DFT. Three theoretical model surfaces with a (3x1) periodicity were selected; one unreconstructed surface, and two with either a missing row (MR) or an added row (AR) of Co atoms along [0001], to represent the reconstruction (Figure 1). The calculations were performed with the Vienna ab initio simulations package (VASP) [3].

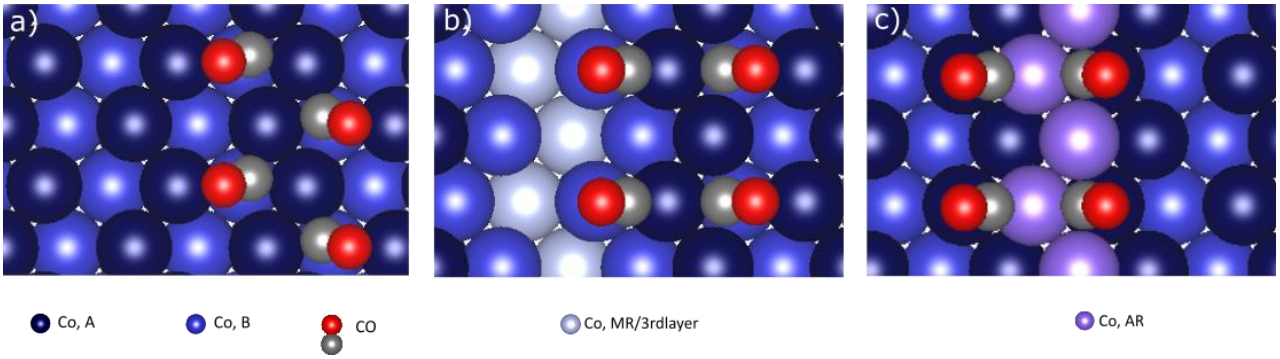

Figure 1: the calculated preferred adsorption geometries of 4 CO on (3x2) model surfaces of Co(11-20) (a) unreconstructed (b) MR and (c) AR.

Slightly higher stability was obtained for CO on the reconstructed surfaces, with CO in coordination with the added row yielding the lowest calculated adsorption energies. Furthermore, lower desorption temperature for CO adsorbed on an unreconstructed surface than from a reconstructed surface was found from HRPES and TPD measurements. Transition state calculations with climbing image nudged elastic band (CI-NEB) [4] were performed to investigate the removal of a Co atom from the topmost layer and its mobility across the surface. These results as well as effects of coverage will be discussed in relation to the experimental data.

References:

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