CO methanation over supported bimetallic Ni-Fe catalysts: From computational studies towards catalyst optimization - DTU Orbit (12/08/2019)

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DFT calculations combined with a computational screening method have previously shown that bimetallic Ni-Fe alloys should be more active than the traditional Ni-based catalyst for CO methanation. That was confirmed experimentally for a number of bimetallic Ni-Fe catalysts supported on MgAl2O4. Here, we report a more detailed catalytic study aimed at optimizing the catalyst performance. For this purpose, two series of mono and bimetallic Ni-Fe catalysts supported on MgAl2O4 and Al2O3, respectively, were prepared. All catalysts were tested in the CO methanation reaction in the temperature interval 200-300 degrees C, and characterized using elemental analysis, N-2 physisorption measurements, XRD and TEM. Optimization of the catalyst performance was made by varying the Ni:Fe ratio, the total metal loading and the support material. For both support materials, the bimetallic catalysts with compositions 25Fe75Ni and 50Fe50Ni showed significantly better activity and in some cases also a higher selectivity to methane compared with the traditional monometallic Ni and Fe catalysts. A catalyst with composition 25Fe75Ni was found to be the most active in CO hydrogenation for the MgAl2O4 support at low metal loadings. At high metal concentrations, the maximum for the methanation activity was found for catalysts with composition 50Ni50Fe both on the MgAl2O4 and Al2O3 supports. This difference can be attributed to a higher reducibility of the constituting metals with increasing metal concentration. The maximum of the catalytic activity and the highest selectivity to methane were observed for the sample with 20 wt% total metal loading. It appears that it is possible to increase substantially the efficiency of Ni-based methanation catalyst by alloying with Fe. (c) 2007 Elsevier B.V. All rights reserved.

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