Unveiling the role of surface hydroxyl groups on Rh₁/ZrO₂ catalyst for direct methane conversion to methanol

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Surface hydroxyl groups on a single atomic Rh catalyst immobilized on zirconia (Rh₁/ZrO₂) were modified by hydrothermal treatment. The effect of surface hydroxyl groups was investigated for the direct methane conversion to methanol using both O_2 and H_2O_2 as oxidants. As the oxidation state of the surface Rh atom increased with an enhanced amount of hydroxyl groups, higher methane activation was achieved. The amount of H_2O_2 could be reduced with enhanced methanol productivity in the presence of the surface hydroxyl groups. The formation of surface hydroxyl groups by hydrothermal treatment and their disappearance upon reaction were confirmed with diffuse reflectance infrared Fourier transform spectroscopy, indicating that the surface hydroxyl groups participate in the surface reaction.