# Selective Activation of Methane on Single-Atom Catalyst of Rhodium Dispersed on Zirconia for Direct Conversion

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Direct methane conversion into value-added products becomes more important. Due to inertness of methane, cleaving the first C-H bond has been very difficult requiring high reaction temperature on the heterogeneous catalysts. Once the first C-H bond becomes activated, the remaining C-H bonds are successively dissociated on the metal surface, hindering the direct methane conversion into chemicals. Here, a single-atom Rh catalyst dispersed on ZrO2 surface has been synthesized and used for selective activation of methane. The Rh single atomic nature was confirmed by extended X-ray fine structure analysis, electron microscopy images, and diffuse reflectance infrared Fourier transform spectroscopy. A model of the single-atom Rh/ZrO2 catalyst was constructed by density functional theory calculations, and it was shown that CH3 intermediates can be energetically stabilized on the single-atom catalyst. The direct conversion of methane was performed using H2O2 in the aqueous solution or using O2 in gas-phase as oxidants. Whereas Rh nanoparticles produced CO2 only, the single-atom Rh catalyst produced methanol in aqueous phase or ethane in gas-phase.