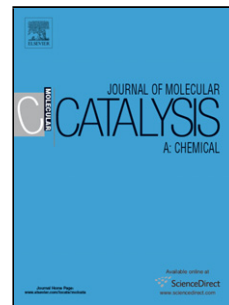


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Title: Gas-phase epoxidation of propylene by molecular oxygen over Ag-CuCl₂/BaCO₃ catalyst with low CuCl₂ doping: Catalytic performance, deactivation and regeneration

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<AT>Gas-phase epoxidation of propylene by molecular oxygen over Ag-CuCl₂/BaCO₃ catalyst with low CuCl₂ doping: catalytic performance, deactivation and regeneration

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<ABS-Head><ABS-HEAD>Graphical abstract

<ABS-P>

<ABS-P><xps:span class="xps_Image">fx1</xps:span>

<ABS-HEAD>Highlights▶

<remove picture pageno 1>Ag-CuCl₂/BaCO₃ catalyst was prepared by reduction-deposition-impregnation method.

<remove picture pageno 1>Ag-CuCl₂/BaCO₃ catalyst with low CuCl₂ doping exhibits better catalytic performance.

<remove picture pageno 1>Epoxidation of propylene over Ag-CuCl₂/BaCO₃ catalyst follows Rideal-Eley mechanism.

<remove picture pageno 1>Molecular oxygen species benefit epoxidation of propylene to propylene oxide.▶▶ Ag-based catalyst is deactivated by coke deposition and can be entirely regenerated.

<ABS-HEAD>ABSTRACT

<ABS-P>Ag-MCl_x/BaCO₃ catalysts with different chloride promoters, prepared by reduction-deposition-impregnation method, were investigated for gas-phase epoxidation of propylene to propylene oxide (PO) by molecular oxygen. Ag-CuCl₂/BaCO₃ catalyst with 360 ppm of Cu and 400 ppm of Cl exhibits the best initial catalytic performance, in which PO selectivity of 71.2% and propylene conversion of 1.3% are achieved, but only PO selectivity of 13.9% is obtained at propylene conversion of 3.2% after reaction for 500 min. The catalytic reaction mechanism over Ag-CuCl₂/BaCO₃ catalyst follows Rideal-Eley mechanism, in which propylene in the gas phase reacts with molecular oxygen species adsorbed on the surface of Ag at the interface in close contact with CuCl₂ to produce PO, and with atomic oxygen species adsorbed on the surface of Ag nanoparticles to produce CO₂ and H₂O. One oxygen atom of molecular oxygen species reacts with propylene to form a PO molecule, and the left insufficient oxygen atoms react with propylene to produce oxygen-containing intermediates

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