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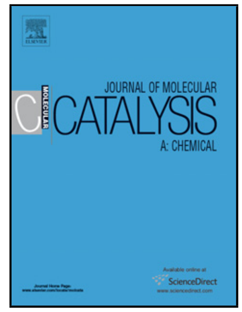


Title: Gas-phase epoxidation of propylene by molecular oxygen over Ag-$CuCl_2$/$BaCO_3$ catalyst with low $CuCl_2$ doping: Catalytic performance, deactivation and regeneration

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<AT>Gas-phase epoxidation of propylene by molecular oxygen over Ag-$CuCl_2$/$BaCO_3$ catalyst with low $CuCl_2$ doping: catalytic performance, deactivation and regeneration

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<ABS-Head><ABS-HEAD>Graphical abstract
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<ABS-HEAD>Highlights►
<remove picture pageno 1>Ag-$CuCl_2$/$BaCO_3$ catalyst was prepared by reduction-deposition-impregnation method.

<remove picture pageno 1>Ag-$CuCl_2$/$BaCO_3$ catalyst with low $CuCl_2$ doping exhibits better catalytic performance.

<remove picture pageno 1>Epoxidation of propylene over Ag-$CuCl_2$/$BaCO_3$ 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-$MCl_x$/$BaCO_3$ 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-$CuCl_2$/$BaCO_3$ 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-$CuCl_2$/$BaCO_3$ 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 $CuCl_2$ to produce PO, and with atomic oxygen species adsorbed on the surface of Ag nanoparticles to produce $CO_2$ and $H_2O$. 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