Structure to catalytic activity relationship of Ag nanoclusters confined in LTA zeolite for CO oxidation

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Silver nanoclusters (Ag_n, n<10) have recently received considerable attention due to their peculiar optical, electronic, and physicochemical properties.[1] Silver nanoclusters can be confined inside the nanocages of zeolites and as a result, their size, shape, charge and nuclearity can be precisely controlled, having such properties a high influence in their catalytic and optical properties.[2,3] Silver clusters stabilized in LTA zeolites are highly luminescent materials with emission spanning over the visible spectrum with external quantum efficiencies up to 69%.[4]

In this study, the structures and optical properties of Ag clusters in LTA zeolites during CO oxidation reaction were investigated using a combination of spectroscopic (UV-Vis, DRS, PL), and X-ray based techniques (XAFS). The high catalytic activity of Ag clusters in the first reaction cycle decreases considerably in the second cycle. The strong luminescence of Ag clusters in LTA (~720 nm emission maximum) observed at the initial stages of the catalytic reaction is quenched after the second reaction cycle, forming non luminescent Ag species. The structure and local environment of catalytically active and luminescent Ag clusters confined in LTA zeolites determined by XAFS consist of octahedral Ag_6 species located inside the sodalite cages. The remarkable concomitant decrease of their catalytic activity and luminescent properties after two consecutive CO oxidation reaction cycles is attributed to the formation of stronger interactions between Ag atoms forming the clusters and oxygen atoms of the zeolite framework.

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