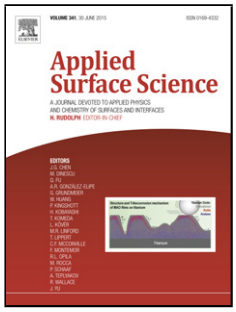

Title: A Study on the Morphology and Catalytic Activity of Gold Nanoparticles by the Kinetic Monte Carlo Simulation

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Highlights

Structural evolution of Au nanoparticles on substrates is simulated by kinetic MC.

Effect of temperature and metal-substrate interaction on the morphology is examined.

Activity to oxidize CO correlates with the number of top edge sites of Au particles.