

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Oxidation of CO on various Fe₂O₃ surfaces: A Theoretical Study

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Virginia Commonwealth University, B.V. REDDY, Philip Morris USA — Recent experiments indicate that Fe₂O₃ nanoparticles can oxidize CO to CO₂ in the absence or presence of O₂. Depending on the size and experimental conditions, a Fe₂O₃ nanoparticle can have different faces that correspond to bulk surfaces of various orientations; which in turn can affect the catalytic activity of the nanoparticle. Hence, an understanding of the reaction pathways, transition barriers, and the feasibility of CO oxidation on bulk surfaces of different orientations are critical to optimize the selection of nanoparticles. Theoretical investigations of the oxidation of CO on various Fe₂O₃ surfaces using gradient corrected density functional approach has been carried out. BPW91 functional form and double numeric basis set (DNP), as implemented in Dmol3 code are employed here. Different Fe₂O₃ (corundum) faces/surfaces are modeled by a cluster where the edge atoms are saturated by H atoms to simulate the effect of the infinite surface. Results corresponding to the reaction of CO with (100) and oxygen terminated (0001) surfaces at various surface sites; oxidation of CO, both in the presence as well as absence of oxygen, will be presented and discussed.

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Date submitted: 23 Nov 2005

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