

Abstract Submitted
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A Density Functional Theory study of Cobalt nanoparticle catalyst for Fischer-Tropsch Synthesis¹ CHANDANA GHOSH, Department of Chemical Engineering, University of South Florida — In the Fischer-Tropsch synthesis Cobalt nanoparticles are widely used as catalysts in which the reaction of Carbon Monoxide and Hydrogen form hydrocarbons. Particle sizes in the range of 6-8 nm have shown to exhibit maximum catalytic activity which is attributed to their surface area and their ability to stabilize steps. Using ab-initio electronic structure calculations based on the density functional theory we study the energetics of adsorption and dissociation of Carbon Monoxide on various particle morphologies and coverages including flat and stepped surfaces and particles with a separation of a few angstroms. The local density of states will be calculated for the various configurations. This study will provide an in-depth understanding of the energetics of adsorption and dissociation of Carbon Monoxide on Cobalt particles and for the various coverages and the particle configurations that lower the dissociation barrier as well as the preferred adsorption sites of the atoms that give the lowest energy for the various particle geometries.

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