

Abstract Submitted
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INS studies of Cobalt-Copper Catalyst for the Conversion of Syngas to Higher Oxygenates¹ PHILLIP SPRUNGER, ZI WANG, MATTHEW PATTERSON, RICHARD KURTZ, JAMES SPIVEY, Louisiana State University — Cobalt-copper catalysts have been proposed for the synthesis of ethanol and higher oxygenates as a substitute of Rh and other high-cost noble metal catalysts. Two types of sites with atomic proximity are needed to form higher oxygenates: one to dissociate CO and a second to insert CO to the intermediates to form the CH_xCO intermediate. Metallic cobalt is responsible for CO dissociation, while the nature of the site for CO insertion is still under study. We have utilized inelastic neutron scattering (INS) at the VISION beamline at SNS to probe intermediate surface species of this cobalt-copper catalyst. This unique technique allows for elucidation of mechanistic details of the CO insertion and subsequent CH_xCO intermediate formation on the metal surfaces (Co⁰, Co₂C and/or Cu⁰). In addition to XRD and EXAFS which show a unique surface Co-C carbide formation, a combination of both INS and computational modeling indicate that the active site for CH_xCO intermediates.

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