Abstract Submitted
for the TSS10 Meeting of
The American Physical Society

A DFT study on Molybdenum/di-Sulfide-Cobalt/Sulfide interface to understand the promotion effect in nano-structured catalytical materials MANUEL RAMOS, MRTI-UTEP, GILLES BERHAUT, IRCELYON-CNRS; France, BRENDA TORRES, MRTI-UTEP, DOMINGO FERRER, MERC UT-Austin, RUSELL CHIANELLI, MRTI-UTEP — Previous studies done to understand promotion effect and structure/function in unsupported catalyst show that d-electrons plays an important role promoting catalytical active sites at the edges of MoS_2 forming so-called CoMoS phase. Information about how Co-Mo acted together is under discussion still and has been approached by meaning of Density Functional Theory (DFT) indicating that hydrodesulfurization takes place at the MoS_2 edge when promoted with Co, several technical papers reports lattice parameter, particle size, crystallographic structure and promotion by meaning of STM on MoS_2/Au. We present here most recent results on DFT calculations using CASTEP for MoS_2/Co nano-structure in order to explain promotion effect as observed by High Resolution TEM on MoS_2/Co nano-structured materials.*(Authors dedicated this research work to:* ***Edward I. Stiefel*** *for his immense contributions to the field of transition metal catalysis while at ExxonMobil research labs.).*

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Date submitted: 08 Mar 2010 Electronic form version 1.4