

Abstract Submitted
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Computational modeling on molybdenum sulfide grain boundary interfaces¹ MANUEL RAMOS, UTEP, RUSSELL R. CHIANELLI TEAM², MIGUEL CASTRO-COLIN TEAM, DOMINGO FERRER TEAM, BRENDA TORRES TEAM, JOHN MCCLURE TEAM — Since discovery of the CoMoS phase in catalysis, many investigations had been conducted in order to understand its intrinsic chemical-physical properties. The CoMoS phase is important because it posses strong catalytical properties. Up to now some models exist in order to explain a mechanism of why this phase is created on a catalyst. Those models are “cherry model” which assumes that Co atoms start nucleating on MoS₂ at the edges, other model like “decoration” states that Co atoms are added on the MoS₂ edges in a decoration form, however even when those two mentioned models are based on density functional calculations (DFT), they lack of explain how two different interfaces meet (MoS₂/Co₉S₈, or MoS₂/Ni₃Co₆) in a bulk catalyst, this lacking of information provided by the models could be attribute to the fact that they are made to explain specific cases, such as small particles (*Hexagonal truncated, Nano-octahedral and Triangular prism*) containing around 10⁵ atoms as much. This work presents computational calculations using Cerius2 molecular software to model based on DFT methods the CoMoS and NiMoS interfaces. Obtain information will be compared with results obtained by HRTEM.

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