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Mapping MoS$_2$-Co Catalytic Nanostructures using HRTEM and TEM Simulations

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Understanding the morphology of catalytically active materials has been approached in past decades with very good results when using field electron microscopy in scanning and transmission modes. In the past some simulated TEM measurements for alumina supported molybdenum sulfide AlO$_2$/MoS$_2$ provided some insights about molecular structure in those catalytic layered transition metal sulfides (LTMS). However, due to resolution, color enhancement, tomography and other factors, sections of those materials observed under TEM do not resolve the structure by itself; in particular for localization of cobalt atoms for MoS$_2$ unsupported catalyst. This work concludes a lattice distance of 0.62 nm and 0.299 nm for Mo-S and Co respectively; results presented here were obtained using experimental HRTEM and molecular modeling to produced TEM simulations, which performs a full dynamical calculation by multi-slice method with a slice thickness of 0.1 Å and using projected potential $f(U) = \sum_{i=1}^{N} a_i e^{-b_i U^2}$, where $a_i$ and $b_i$ are coefficients to be determined. The variable $U = (u, v, w)$ is used to represent coordinates in reciprocal space (Fourier space) quantities (spatial frequencies). $f(U)$ is the atomic dispersion factor.