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Correlation of oxygen defects with surface Lewis acidity and catalytic properties of hybrid MoO₃/SBA-15 catalysts

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There are many structural defects or lattice vacancies in the surface of solid materials. From the surface sciences and catalysis points of view, these cationic or anionic defects are active centers for reactant adsorption and surface reactions. Investigation on structural defects and their correlation with reaction activity may provide new insight into the understanding of catalytic behaviors. In this work, a set of MoO₃/SBA-15 mesoporous hybrid catalysts were characterized with a variety of spectroscopic techniques and their crystalline structures were refined with Rietveld method. Oxygen defect concentration, crystallite size, phase composition, surface acidity, mesoporous regularity and textural properties were reported. Both α -MoO₃ and β -MoO₃ phases coexisted but α -MoO₃ was predominated. Oxygen defects were created in the orthorhombic structure and its concentration decreased as MoO₃ content increased. All the MoO₃/SBA-15 catalysts chiefly contained a big number of Lewis acid sites originating from oxygen defects in MoO₃ crystals. In the absence of formic acid, the oxidation of 4,6-dibenzothiophene in a model diesel was almost proportional to the number of Lewis acid sites of the catalysts. In the presence of formic acid, 4,6-dimethyldibenzothiophene (4,6-DMDBT) oxidation was significantly affected by the formation of surface peroxometallic complex and Lewis acidity. Formic acid addition could improve the oxidative desulfurization (ODS) efficiency by promoting peroxometallic complex formation and enhancing oxidant stability. Under the optimal reaction condition using the best 15 and 20 wt% MoO₃/SBA-15 catalysts, more than 99% 4,6-DMDBT could be removed at 70°C within 30 min. This work confirmed that 4,6-DMDBT oxidation is a texture and particle size sensitive and Lewis acidity dependent reaction. This work also shows that crystalline structure refinement combination with experiments can gain new insights in the design of heterogeneous nanocatalysts and help to better understand the catalytic behavior in the oxidative desulfurization reactions.

Recent Publications

1. González J, Wang J A, Chen L F, Manríquez M E and Dominguez J M (2017) Structural defects, Lewis acidity and catalysis properties of mesostructured WO₃/SBA-15 nanocatalysts. *Journal of Physical Chemistry C* 121(43):23988–23999.
2. González J, Wang J A, Chen L F, Manriquez M, Limas R, et al. (2016) Surface chemistry and catalytic properties of VOX/Ti-MCM-41 catalysts for dibenzothiophene oxidation in a biphasic system. *Applied Surface Science* 379:367–376.
3. Ramos J M, Wang J A, Arellano U, Chen L F, Ramirez Sebastian S P and Sotelo Boyás R (2015) Oxidative removal of dibenzothiophene from model diesel fuel using CoMo/SBA-15 catalysts. *Catalysis Communications* 72:57–62.
4. Brezesinski T, Wang J, Tolbert S H and Dunn B (2010) Ordered mesoporous α MoO₃ with iso-oriented nanocrystalline walls for thin-film pseudocapacitors. *Nature Materials* 9(2):146–151.

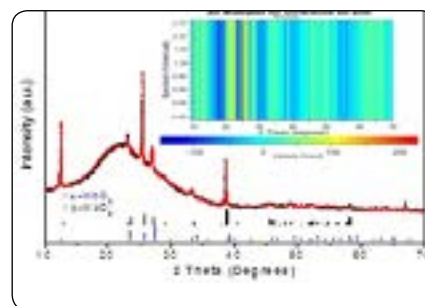


Figure 1: A Rietveld refinement plot for the 20 wt% MoO₃/SBA-15 catalyst.

Biography

Jin An Wang is a full Professor in Chemical Engineering at the National Polytechnic Institute in Mexico City, Mexico. He is a National Researcher of Mexico and a Member of the Mexican Academy of Sciences. He is the Co-Author of more than 160 scientific publications, five patents, Co-Editor of three books in "Advanced Catalytic Materials" and three special volumes in *Catalysis Today*. He served as Chair of the first to fifth International Symposium on New Catalytic Materials. He was a Visiting Professor at Universidad Nacional Autónoma de México, Universidad Autónoma Metropolitana and Worcester Polytechnic Institute in USA. His research interest focuses on the synthesis of new catalytic materials, catalysis for petroleum refining and treatment, catalysis for clean fuel production and environmental catalysis.

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