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EXAFS Structure Determination of Inorganic Cation Template Effects on Nanofibrous Tunnel Structure Manganese Oxide Molecular Sieves

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Beamline(s): X18B

Introduction: Octahedral molecular sieves (OMS) have been widely used in catalysis, batteries, chemical sensors, and other applications. [1] The objective of this experiment is to study local atomic arrangements and chemical states of manganese cations and inorganic cation templates, such as K^+ and Rb^+ , in nanofibrous manganese oxide cryptomelane molecular sieve catalysts using EXAFS. Nanofibrous tunnel structure manganese octahedral molecular sieves have exceptional catalytic properties because of the mixed valent Mn and the unique structural arrangement and shape. Initial work of nanofibrous cryptomelane manganese oxide has been done and characterization results have supported the claim. [2] EXAFS and EXANES will be used to obtain information such as the spatial relationships of metal atoms and surrounding atoms, oxidation states of metal atoms, and the identification of possible amorphous metal oxides, which cannot be readily obtained by other techniques.

Methods and Materials: XANES and EXAFS spectra at the Mn K edge were obtained at beamline X18B. The X-rays were tuned by a Si(111) double crystal monochromators which was detuned slightly to prevent glitches from harmonics. The sample was prepared as a thin layer on Scotch tape that was attached to the slot sample holder. Fluorescence mode was used to obtain the signal.

Results: EXAFS has been used to obtain local environment of Mn. The atomic distances between Mn (or doped metals) and surrounding oxygen atoms have been measured. The comparison of Mn-O distance of M-OMS-2 with different cations confirms that MnOx framework structure was not changed by different cations in the samples. No change of the distances of Mn-O and Mn-Mn in the samples was observed. EXAFS obtains structural information of a short range ordered material. Amorphous metal oxides were not observed in the compounds according to the data. [3]

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References:

- (1). Shen, Y. F.; Zenger, R. P.; DeGuzman, R. N.; Suib, S. L.; McCurdy, L.; Potter, D. I.; O'Young, C. L. *Science*, 1993, 260, 511.
- (2). Liu, J.; Cai, J.; Son, Y.-C.; Gao, Q.; Suib, S. L.; Aindow, M.; *J. Phys. Chem. B*. 2002, 106(38), 9761.
- (3). Ressler, T., Brock, S. L.; Wong, J.; Suib, S. L. *J. Phys. Chem. B*, 1999, 103, 6407.