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XANES Study of Ti Y Zeolite and Related Species

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Beamline(s): X19A

Introduction: Carbon dioxide utilization and selective hydrocarbon oxidation are very important subjects in carbon management strategies to mitigate global climate change [1]. Anpo *et al.* reported that photochemical CO₂ reduction to methanol can be significantly enhanced by the use of titanium oxide species anchored within zeolites [2]. Ti-centered zeolites have also been used as catalysts for the selective oxidation of alkanes and alcohols, and the epoxidation of alkenes [3]. In order to understand the elementary steps of the reactions related to photochemical CO₂ reduction and/or hydrocarbon oxidation in the zeolite, we are exploring the interaction of Ti with the porous framework of the zeolite, and specific interactions of the reactants with Ti and/or the porous framework.

Methods and Materials: Ti Y zeolite was prepared with 10% aqueous (NH₄)₂TiO(C₂O₄)₂ solution with Na Y zeolite, followed by calcination at 350 °C. The Ti K-edge XANES of solid samples was measured in fluorescence mode at 298 K.

Results and Conclusions: Figure 1 shows that the Ti K-edge XANES of calcined Ti Y zeolite (a), uncalcined Ti Y zeolite (b), (NH₄)₂TiO(C₂O₄)₂ (c), and anatase TiO₂ (d). The XANES spectra of these species show several well-defined pre-edge peaks (1s → 3d). The number, position, and relative intensity of these pre-edge peaks provide valuable information about the coordination environment of Ti. As seen from Figure 1, the calcined Ti Y zeolite exhibits one intense pre-edge peak, indicating that the local structure of titanium is in tetrahedral coordination. In the next beam time cycle, we plan to measure EXAFS of these species in order to obtain detailed structural information. These models will also be correlated with the structural models obtained from X-ray diffraction powder profile refinements.

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References:

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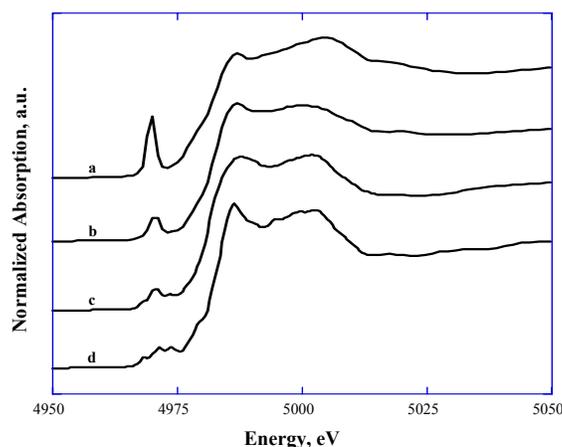


Figure 1. Ti K-edge XANES of calcined Ti Y zeolite (a), uncalcined Ti Y zeolite containing (NH₄)₂TiO(C₂O₄)₂ in the supercage (b), (NH₄)₂TiO(C₂O₄)₂ (c), and anatase TiO₂ (d).