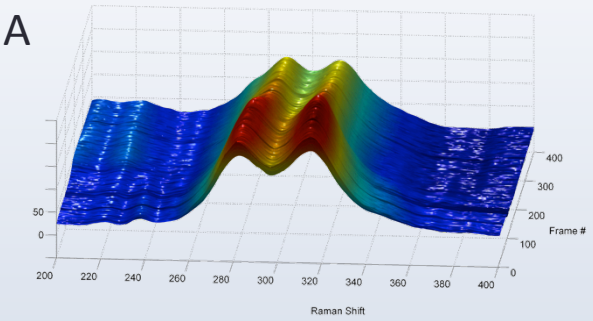
Characterizing Synthesis and Ion Transport in Microporous Mixed-Polyhedral Frameworks

Aaron J. Celestian, Geography and Geology, Western Kentucky University

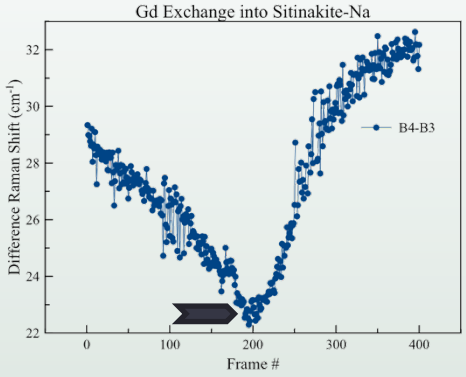
Zorite, sitinakite, and umbite are microporous heterosilicates that have been used as catalysts in the petroleum industry. Zorite (also known as ETS-4) and sitinakite (also known as TS or CST) are titanium silicates that are naturally found in hydrothermally altered igneous rocks. Umbite is a naturally occurring zirconium trisilicate. The ion exchange characterization of these materials are being performed because of their historical uses, and their potential for high temperature and selective catalysis. The goal of this research is to detail the cation exchange mechanisms of rare earth elements (REEs: Y, Eu, Gd, Tb) and transition metals (Ni, Cu, Zn). Example analyses are shown to the right.

A



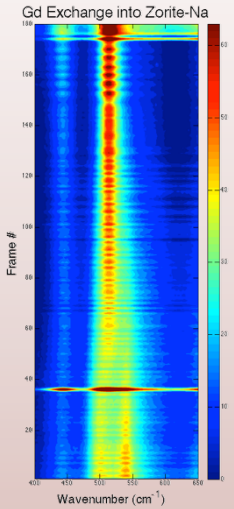
Plot of time-resolved Raman spectra for Gd exchange into sitinakite-Na showing changes in peak positions for the Si-O-Ti and Ti-O-Ti bending modes.

B



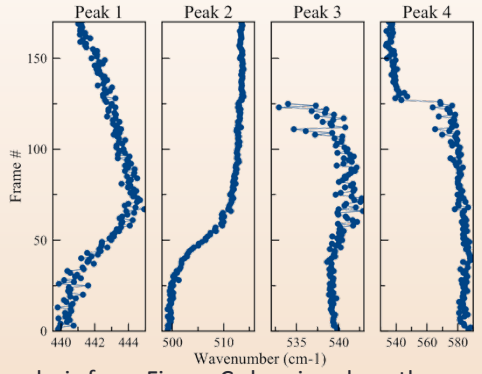
Difference peak analysis from Figure A showing the peaks initially move closer (forming elliptical channels), and then further apart (forming circular channels). Arrow indicates point at which band-gap may change.

C



This data shows the multi-step conformational changes in the channel geometry as Gd exchanges into zorite-Na. In addition to peak migration, high wavenumber fluoresce peaks increase as Gd exchange proceeds. This data, combined with time resolved XRD, and UV-Vis are being used to determine structural properties, kinetics, and band-gap changes.

D



Peak analysis from Figure C showing slow, then rapid peak migration to higher wavenumbers (peaks 1 & 2), and some disappear (peak 3) showing a framework response to the repositioning of Gd as Na is removed from the structure.