NaY Zeolite Templated Carbons

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Hydrogen Storage Background

- Makes use of renewable energy sources
- Reduced dependency on foreign oil
- Reduced environmental impact
- Zero greenhouse gas emissions
- Potentially reduced cost
- Higher efficiency
Hydrogen Storage

- Compressed
- Liquid
- Chemisorption
- Metal Hydrides
- Physisorption
Physisorption

• Advantages
  – Fast kinetics
  – Low pressures
  – Relatively low cost
  – Simple storage mechanisms
  – Fully reversible

• Disadvantages
  – Currently poor gravimetric and volumetric capacities
  – Currently low binding energies requiring very low operating temperatures
NaY Zeolite Templated Carbon

- Prepared at Monash university in Australia
  - NaY zeolite degassed and impregnated with furfuryl alcohol
  - Polymerized in a vertical quartz reactor
  - Carbonized and then chemical vapor deposition with propylene gas
  - Inorganic Supports removed by use of Hydrofluoric acid after heat treatment
  - Extensive filtering and washing with purified water
  - Finally dried in a vacuum at 30c for 24 hours
X-Ray Diffraction

- Probes for any regular structure within the sample by using X-rays to observe the phenomena of diffraction (make sure NaY is gone)
- This is an amorphous material and thus we expect no diffraction patterns (Bragg peaks)
- Only detects very small range structure, sub angstrom to 10s of angstroms
Low Pressure Isotherms

- Sample outgassed overnight at 200°C
- Performed with CO₂, N₂, and H₂ at 294K, 77K, and 77K respectively
- 52.9mg tested on Quantachrome isotherm instrument

N₂ BET SA: 1304 m²/g
H₂ Langmuir SA: 1060 m²/g
Excess Adsorption Isotherms

![Graph showing excess adsorption isotherms for different temperatures.]
High Pressure Isotherms

- Affinity of hydrogen to loading sites decreases with increased loading.
- Decreases with increased temperature.
NG7 Prompt Gamma Activation Analysis

• Each type of atom releases gamma rays of a certain energy level(s) when bombarded with neutrons
• We detect these gamma rays and based on the sensitivity and energy level can determine the approximate proportions of each element.
PGAA Data

Peak Counts: 0.162689 (cps)
Peak Center: 1261.765 (keV)
Elemental Composition (outgassed)

**PGAA Composition**

- **H**: 3198
- **C**: 166000
- **O**: 43478
- **Na**: 270
- **Al**: 194793
- **Cd**: 6.5
- **Y**: 29
- **Pt**: 680
- **F**: 8935
Small Angle Neutron Scattering
• Detects long range structure anomalies 10s-1000s Å
• Log log scale slopes of Q suggest different types of structures
• Consistent with results gained from other instruments

Q^{-1} = one dimensional pore
Q^{-2} = two dimensional pore (two planes)
Q^{-4} = smooth curved surface
NG2 High Flux Backscattering

- High Flux
- High Resolution
- Small Q range
- Detects slow movements
HFBS Data

Templated Carbon HFBS

Temperature (K)

Intensity

- 1.0 wt%
- bare material
- 0.5 wt%
NG4 Disk Chopper Spectrometer

- High Flux
- High Q
- Low resolution
- Detects fast and slow hydrogen movements
0.5 wt% H$_2$ in Na-Y Templated carbon
0.5 wt% H$_2$ in Na-Y Templated carbon

Q-cut [1 - 2]

\[ E_A = -0.58(7) \text{ kJ/mol} \]

\[ E_A = -0.81(3) \text{ kJ/mol} \]
Activation energy = 0.81 kJ/mol

Thin Lorentzian = 0.58 kJ/mol

Compares to
- nanotubes = 0.37 kJ/mol
- Solid H₂ = 1.9 kJ/mol
- Liquid H₂ = 0.37 kJ/mol
- Zeolite 13X = 0.515 - 1.99 kJ/mol
- XC-72 = 1.03 kJ/mol

Fits
- 10K resolution (delta)
- Lorentzian (wide)
- Lorentzian (thin)
- Flat background

Wide lorentzian corresponds with fast movement
Thin corresponds with slow movement

Additional Analysis
BT4 Data

- Quantum J=0-1 peak @14.7 meV
- Broad recoil
- H₂ being knocked off of sites by incident neutrons
- Background subtracted (only hydrogen)
And it was the best summer ever!