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Environmental Materials: From Structures to Functionalities

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DOE Office of Civilian Radioactive Waste Management

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Radionuclides Responsible for Peak Dose in the First 100,000 Years

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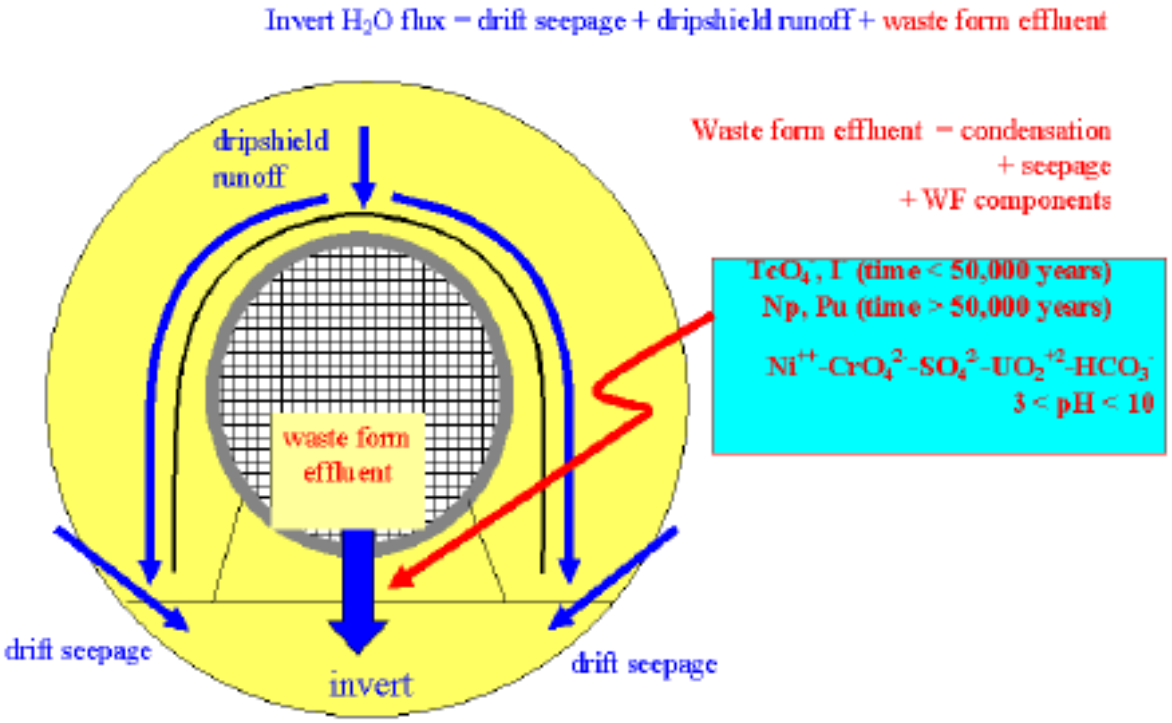
Release of Waste form effluent from the Waste package to the Invert



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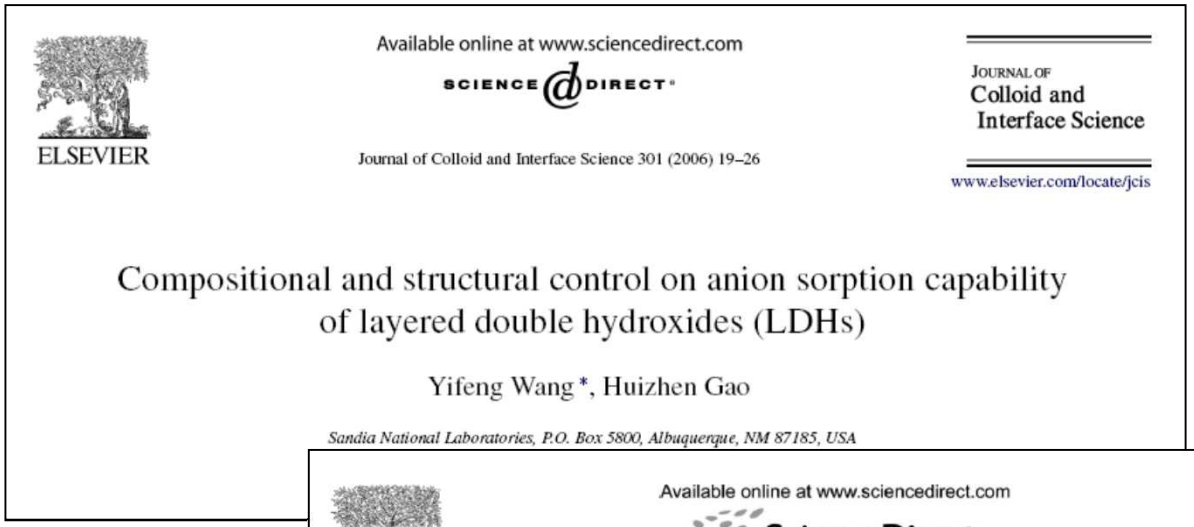

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Compositional and structural control on anion sorption capability of layered double hydroxides (LDHs)

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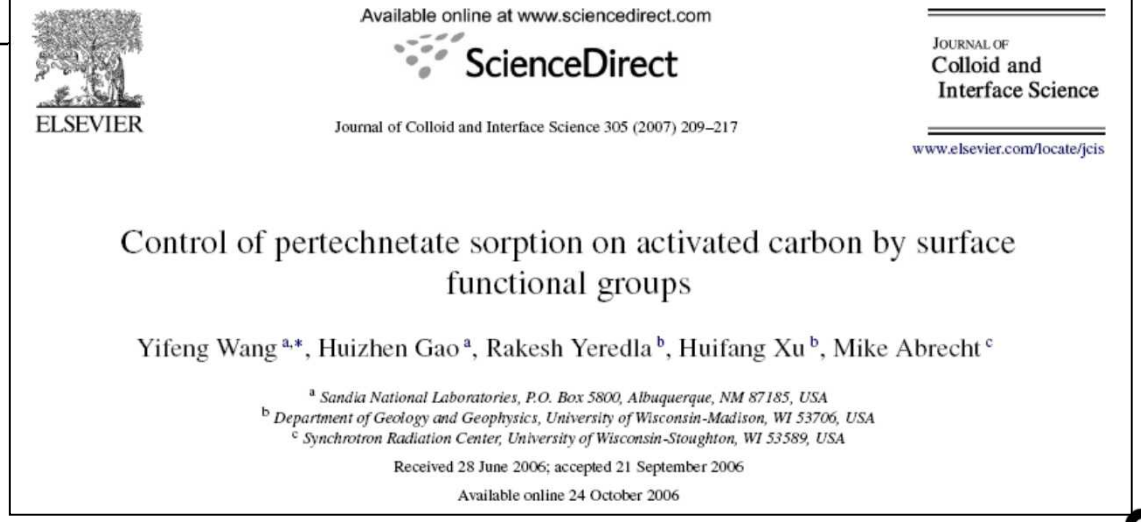

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Control of pertechnetate sorption on activated carbon by surface functional groups

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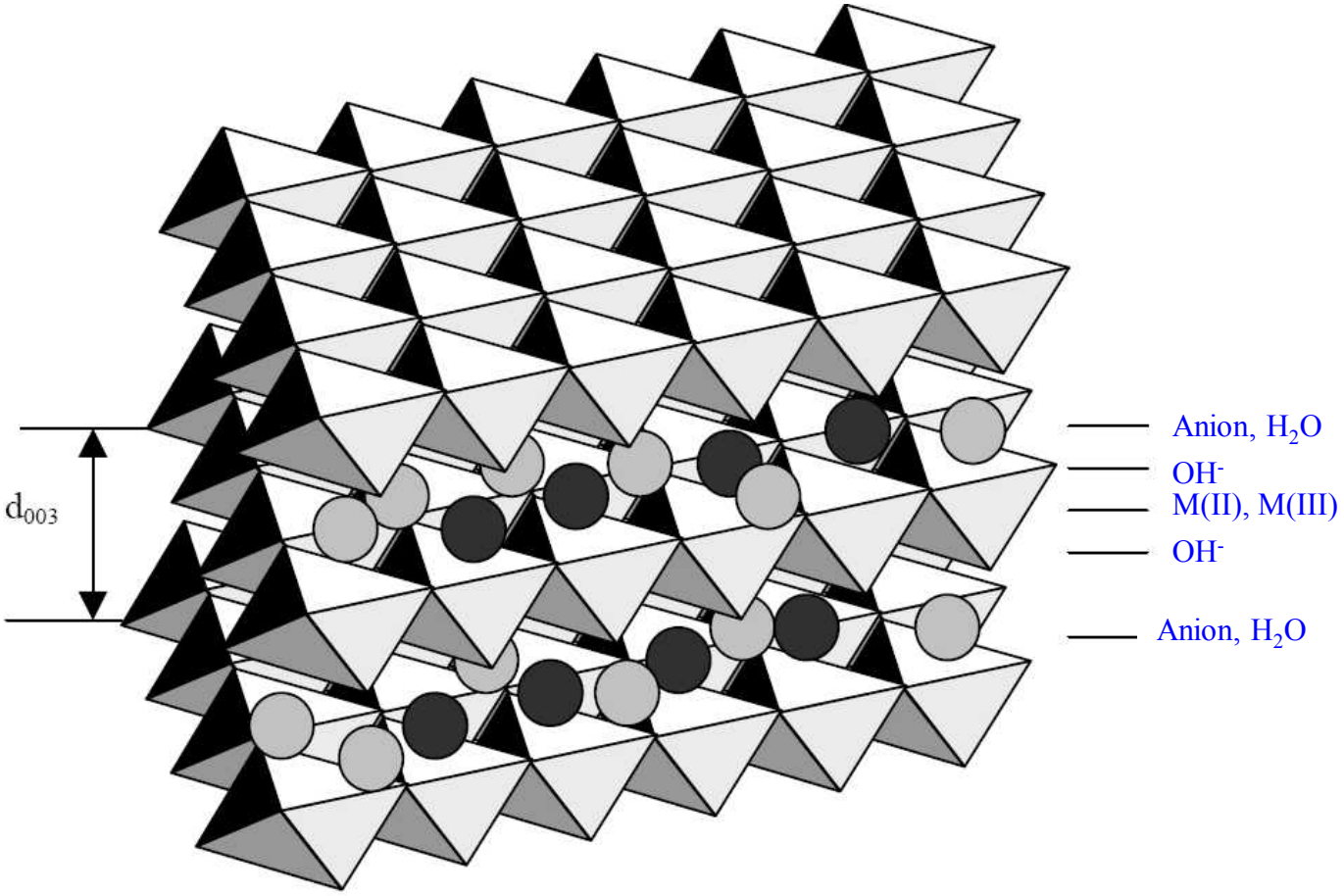
Structure of layered double hydroxide



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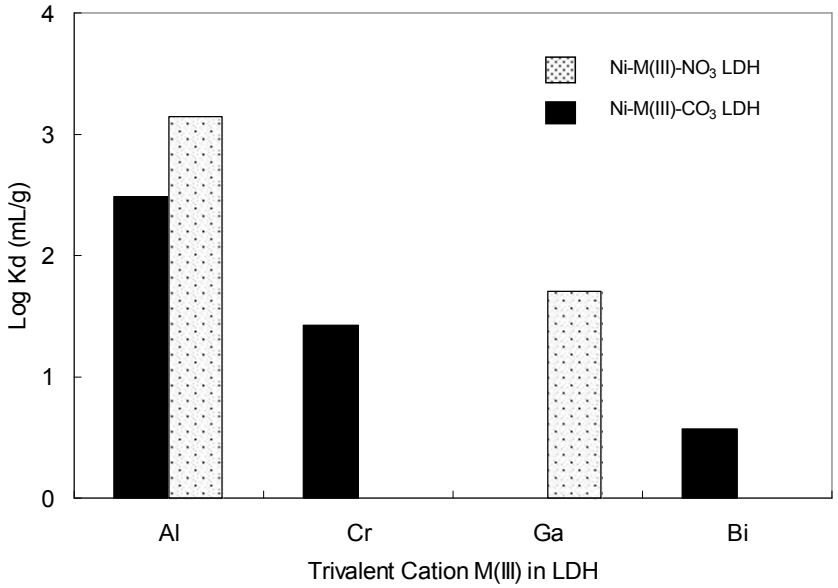
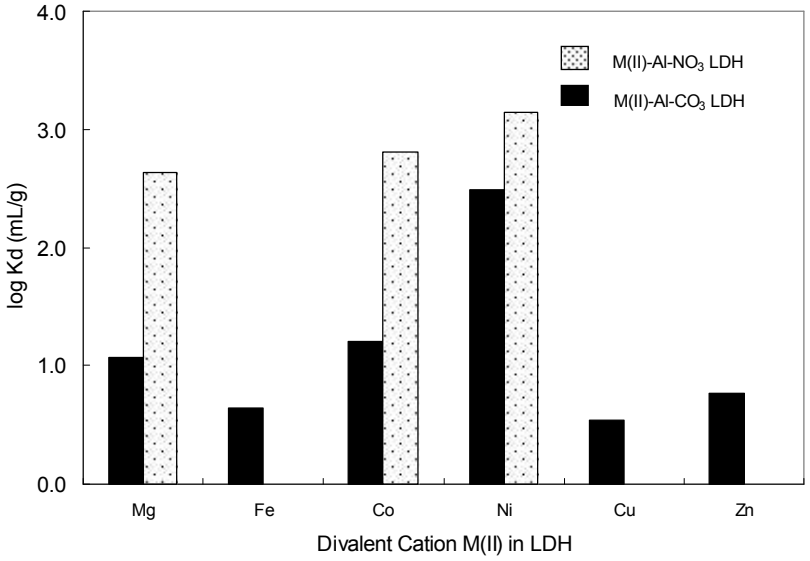
Compositional manipulation





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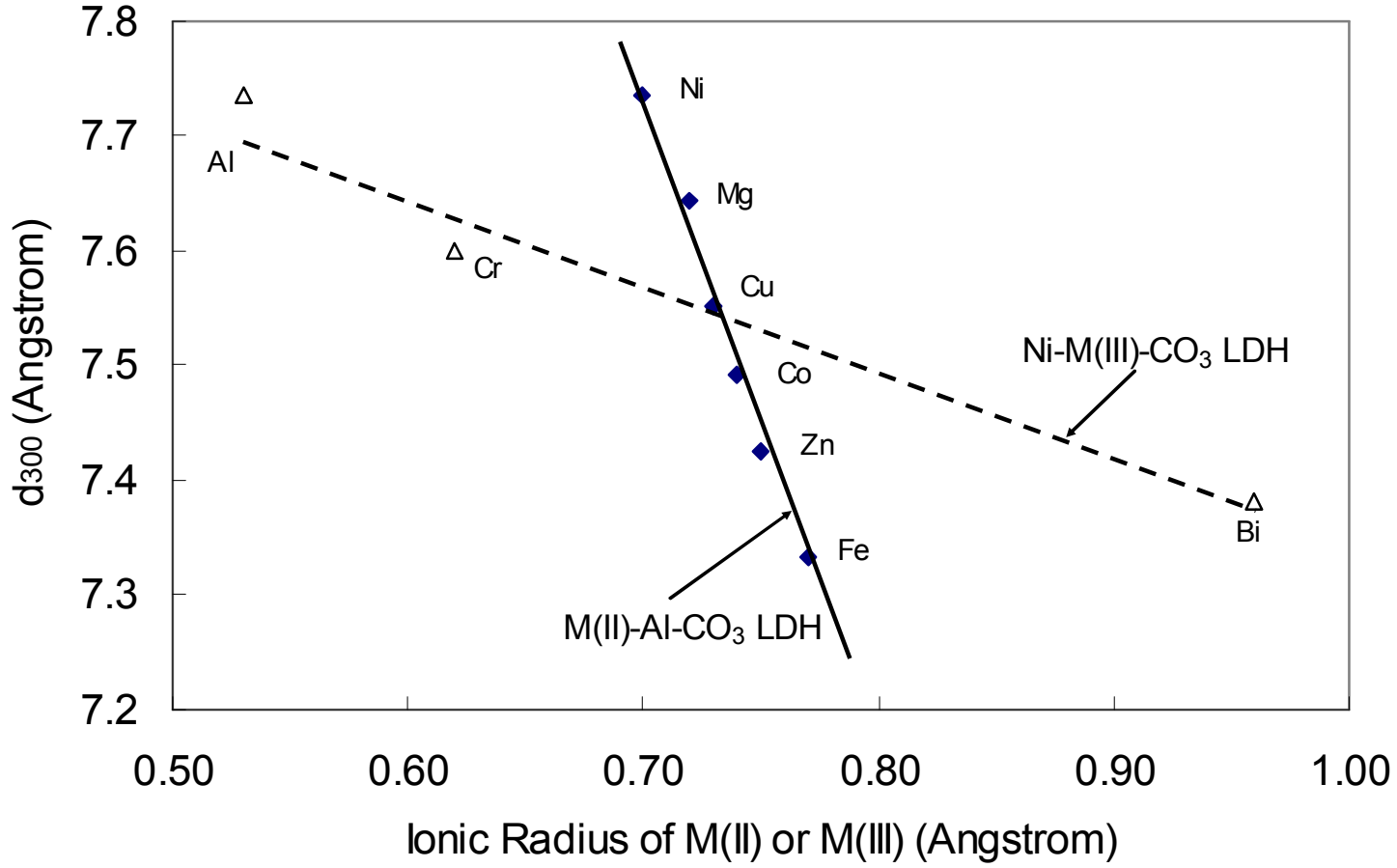
Structural Manipulation



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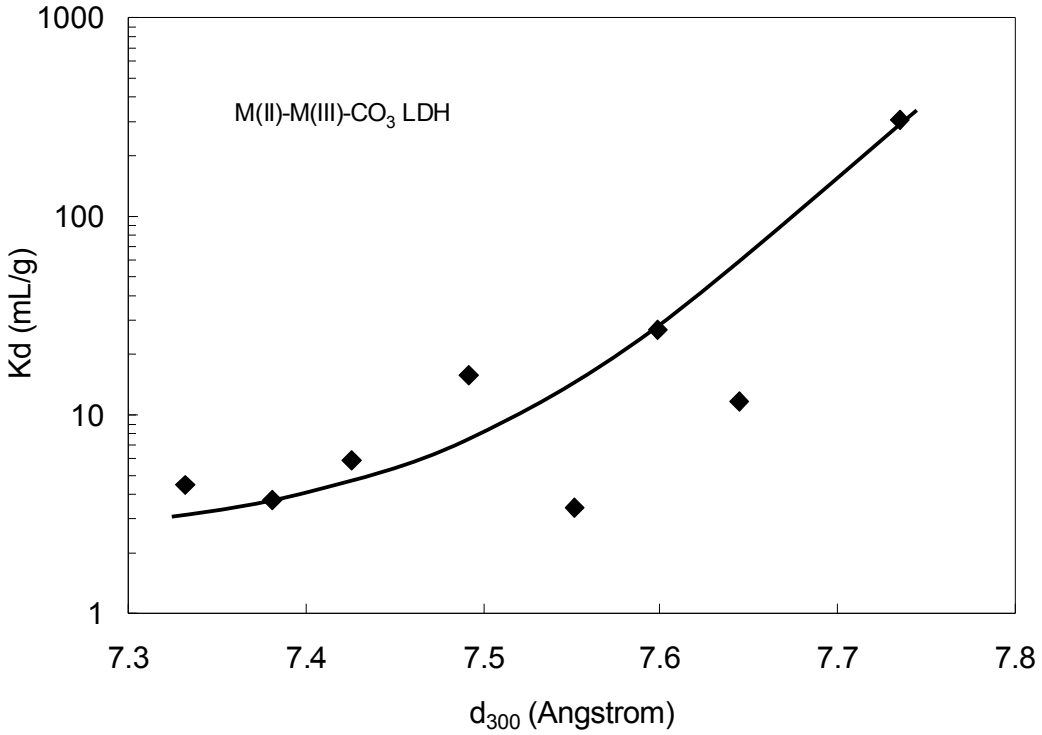
Structural Manipulation (cont.)



Sorption capabilities of M(II)–Al LDH materials for pertechnetate (TcO_4^-)

M(II)	pH	K_d (mL/g)	K_d (mL/g) corrected to pH of 8.0
		M(II)–Al–CO_3 LDH	M(II)–Al–CO_3 LDH
Mg	9.4	4	12
Fe	8.5	3	4
Co	7.7	20	16
Ni	8.5	209	307
Cu	7.8	4	3
Zn	8.5	4	6
Cd	8.1	3	3
		M(II)–Al–NO_3 LDH	M(II)–Al–NO_3 LDH
Mg	9.1	187	435
Co	8.0	631	631
Ni	7.9	1501	1390
		M(II)–Al–SO_4 LDH	M(II)–Al–SO_4 LDH
Ni	6.8	Not detectable	~0
Cu	7.0	Not detectable	~0

Note. M(II)/Al = 3:1 for all materials.

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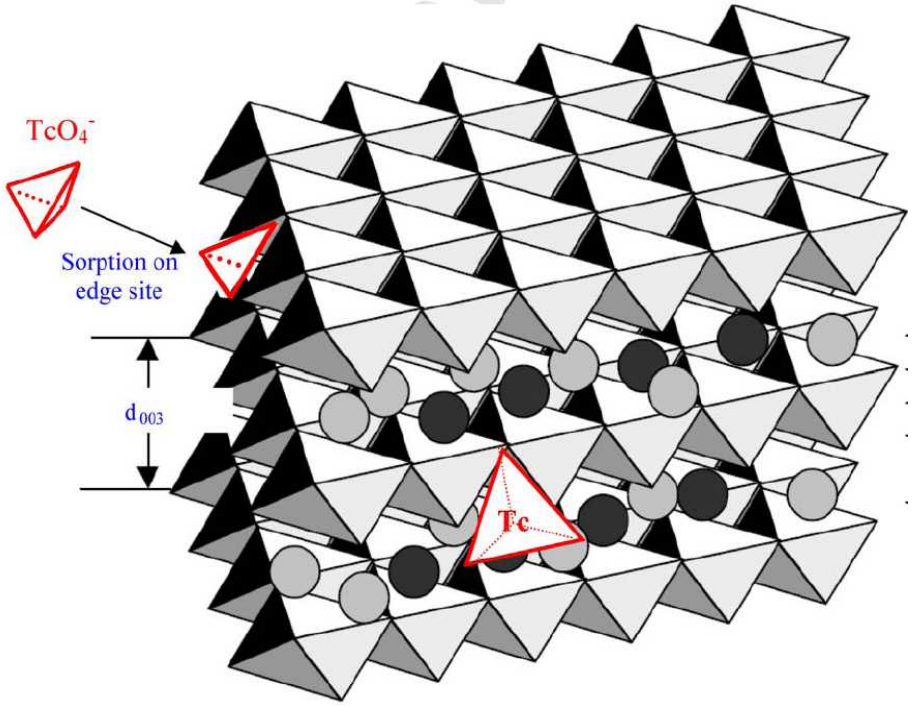
Cage Effect



Maximum TcO_4^- sorption could be reached when the basal spacing is just large enough to fit a pertechnetate anion into a cage space at the edge of LDH layers.

What are activated carbons?

- **Made from a raw material**
  - **Wood, lignite, peat, or coal**
- **Two-stage process:**
  - **Carbonization**
    - **L-carbon: Carbonized at temperature 200 – 400 ^{o}C in air**
    - **H-carbon: Carbonized at temperature (up to 1200 ^{o}C) in inert atmosphere**
  - **Activation**
    - **Resulting chars subsequently subjected to partial gasification at temperature up to 900 ^{o}C with H_2O steam or CO_2**

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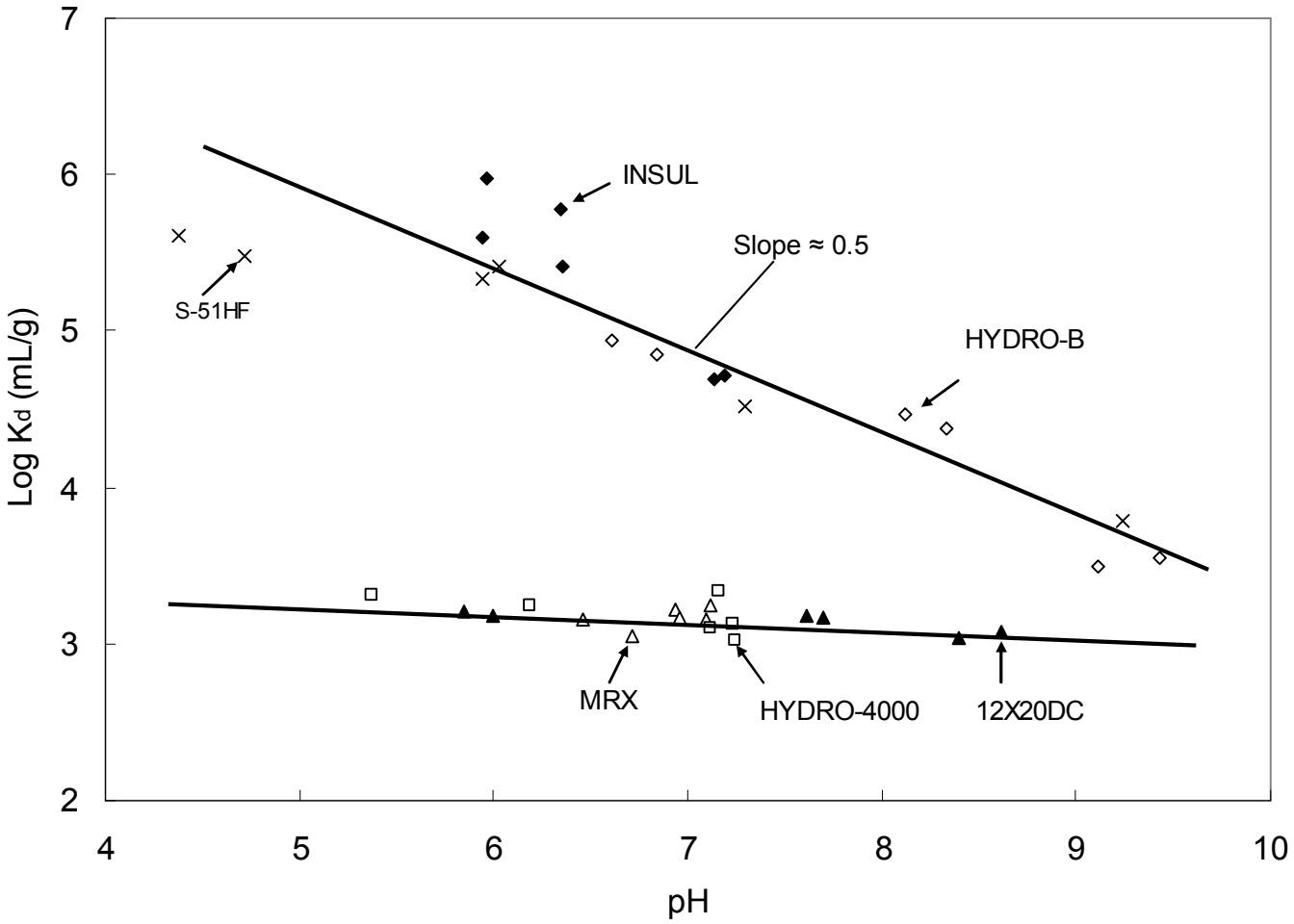
Surface areas and pore sizes of activated carbons

Activated carbon	Surface area, m^2/g	Average pore size nm	Total volume cc/g
INSUL	489	4.6	0.56
HYDRO-B	468	4.3	0.50
HYDRO-4000	750	4.1	0.76
12X20DC	538	4.9	0.66
MRX	557	5.4	0.76
S-51HF	640	4.8	0.77

Sorption of pertechnetate on activated carbons



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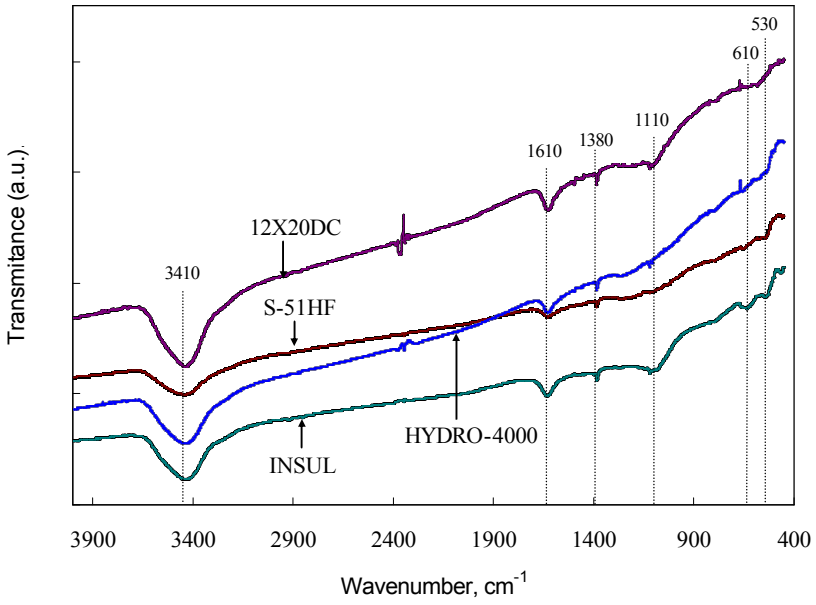
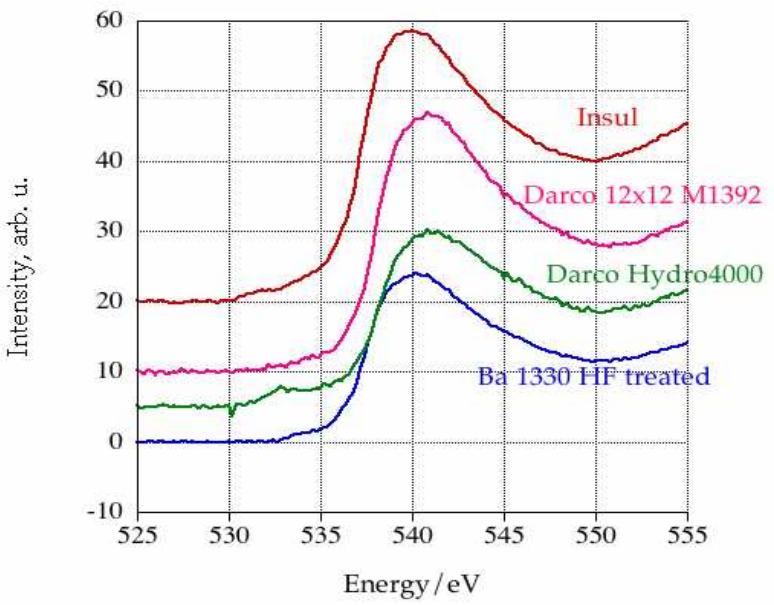
Spectroscopic analyses of activated carbons



FTIR



XPEEM

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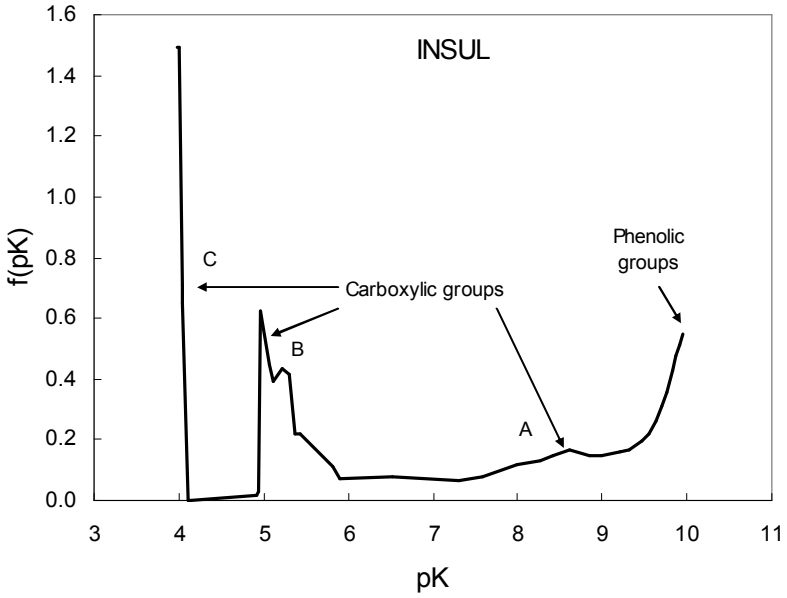
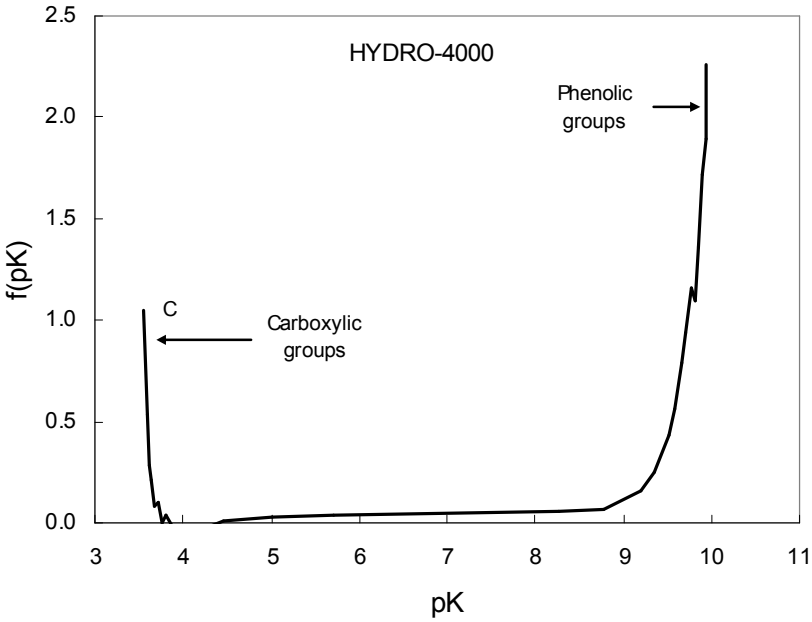
Surface acidity of two groups of activated carbons



High Tc sorption capability



Low Tc sorption capability

Note: All tested materials from the same source

Plenty of room for material engineering by controlling activation process!!!

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Engineered Invert Materials

- High sorption capability (Kd > 500 mL/g)
  - Most existing anion getters: Kd < 500 mL/g
- Stability and longevity
  - Sulfide minerals: not stable under oxidizing conditions
- Availability & cost
  - Activated carbons
    - Kd ~ 10^6 mL/g
    - Inexpensive
    - Readily available
    - Thermally stable
  - Layered double hydroxides
    - In-situ formation (Cr, Al, Ni) (ms. in preparation)

Environmental Materials: From Structures to Functionalilities

- Functional dependence of surface properties on material structures
- Engineering materials for specific applications
- Layered double hydroxides & activated carbon
  - Two idea systems for study of Tc interactions with solid-water interface

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