Georgia Tech | Brook Byers Institute for Sustainable Systems

Summary of Adsorption Work of the Brook Byers Institute for Sustainable Systems

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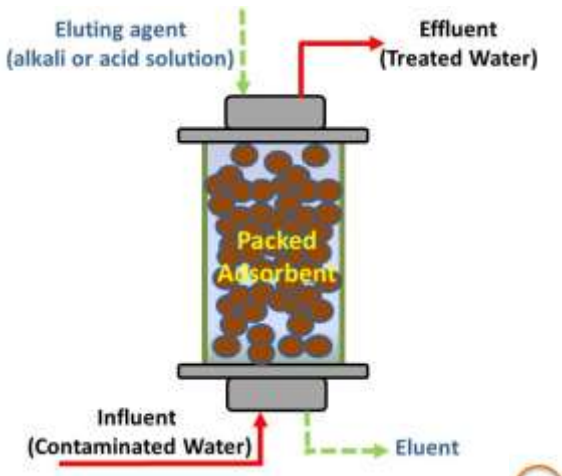
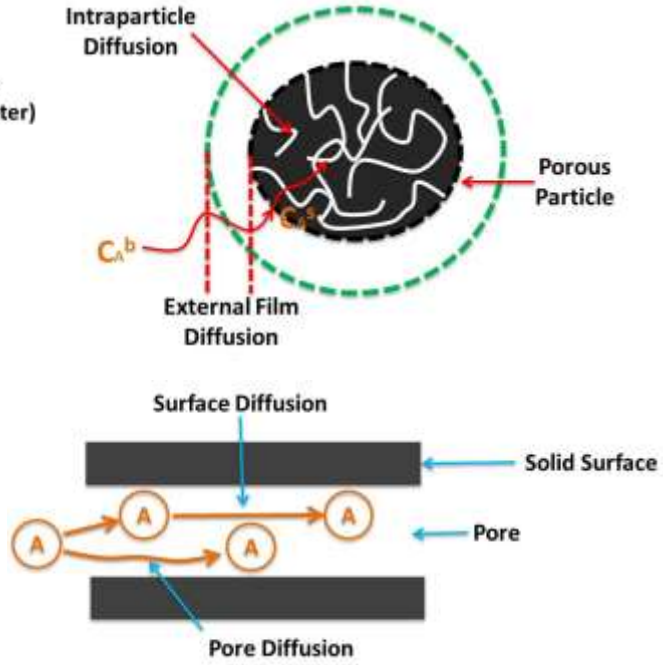
Adsorption Introduction

Adsorption is a mass transfer operation in which substances present in a **liquid phase** are **adsorbed** or **accumulated** on a **solid phase** and thus removed from the liquid. Adsorption processes are used in drinking water treatment for the removal of taste- and odor-causing compounds, synthetic organic chemicals (SOCs), color-forming organics, and disinfection by-product (DBP) precursors. **Granular activated carbon** (GAC) and **powdered activated carbon** (PAC) are the most common adsorbent.





- ***Our Research Directions***
  - Synthesis adsorbents with high adsorption capacity toward target pollutants;
  - Using adsorption isotherm model and adsorption kinetic model to simulate the adsorption experimental data, in order to have overall understanding on the adsorption process;
  - Adsorption field applications predictions using Pore Surface Diffusion Model and Ion Exchange Model
  - Density functional theory (DFT) calculation was applied to unravel the adsorption mechanism

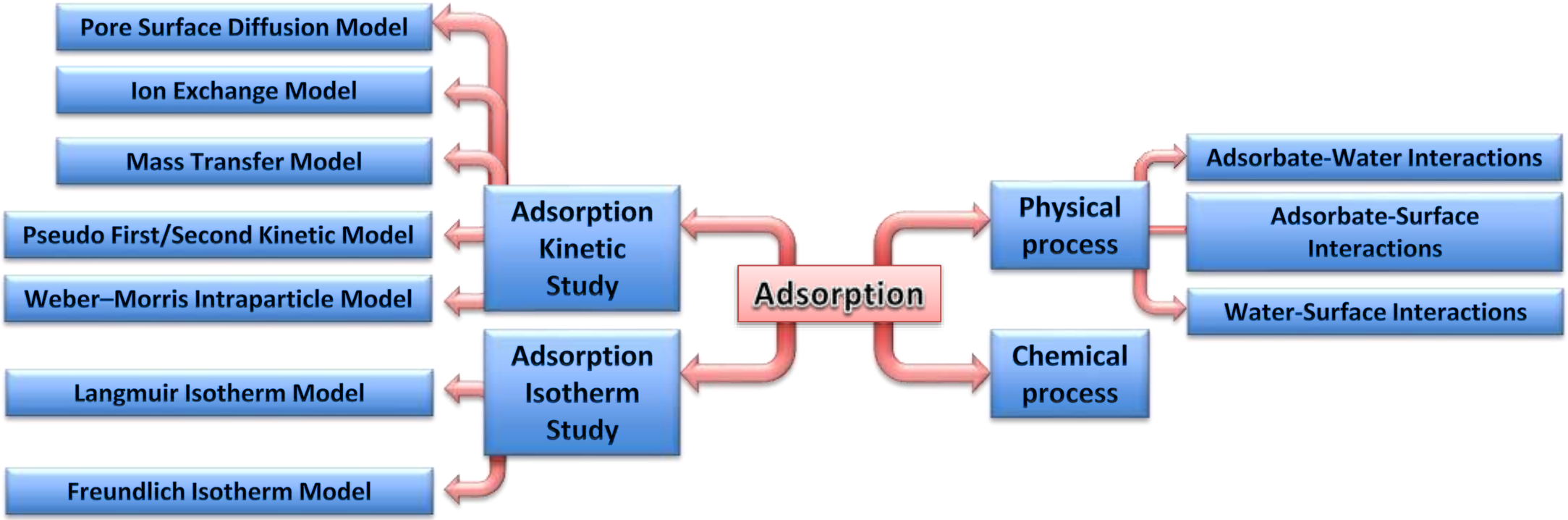
Research Directions

- **Adsorbent** can remove target pollutants on a **molecular level** and the interactions between the adsorbing compound and the adsorbent and how these interactions are impacted by **physical and chemical forces**
- Adsorption performance can be enhanced via **morphology regulation**
- Adsorption mechanism can be further revealed using **extended X-ray absorption fine structure (EXAFS)** and **density functional theory (DFT) calculations**

Essential Performance Indicators:

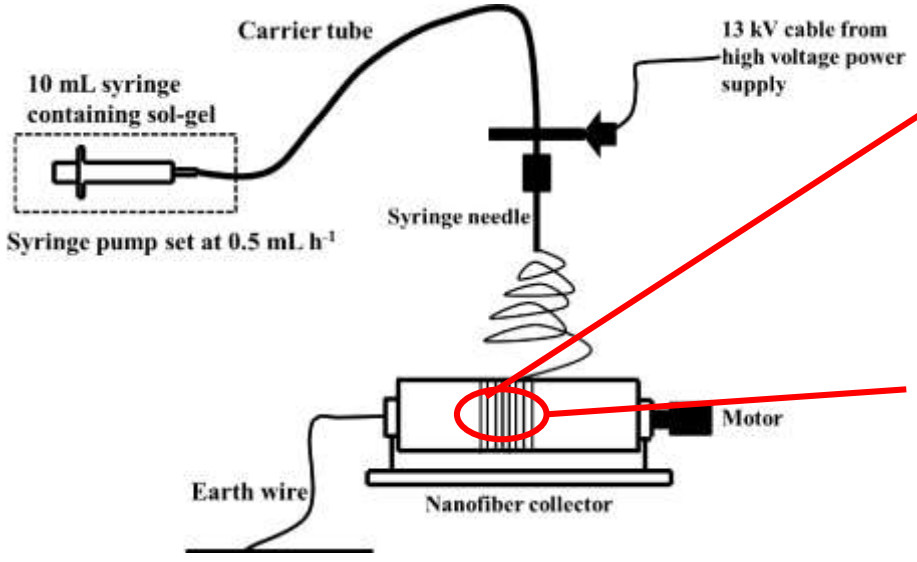
Porosity (Pore size)

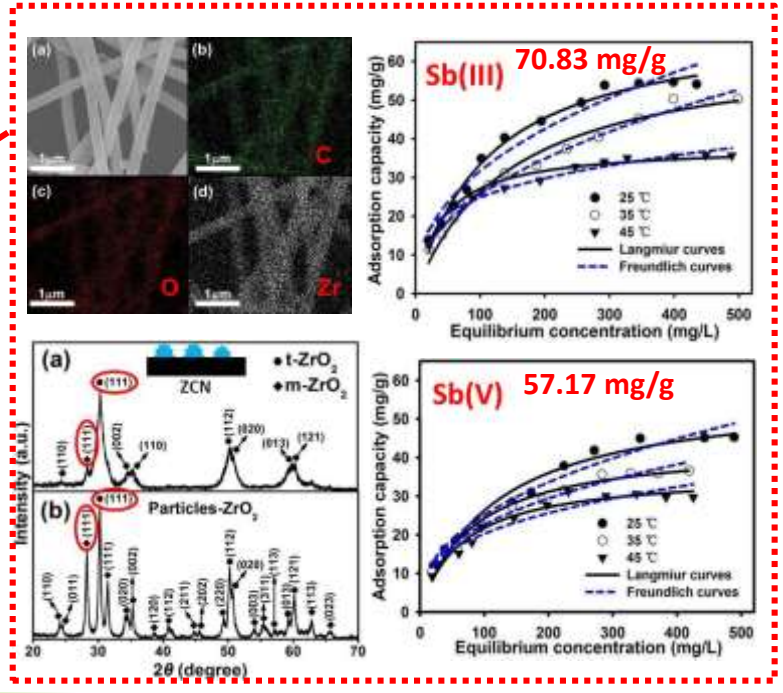
BET surface areas



Our Work on Adsorption Process

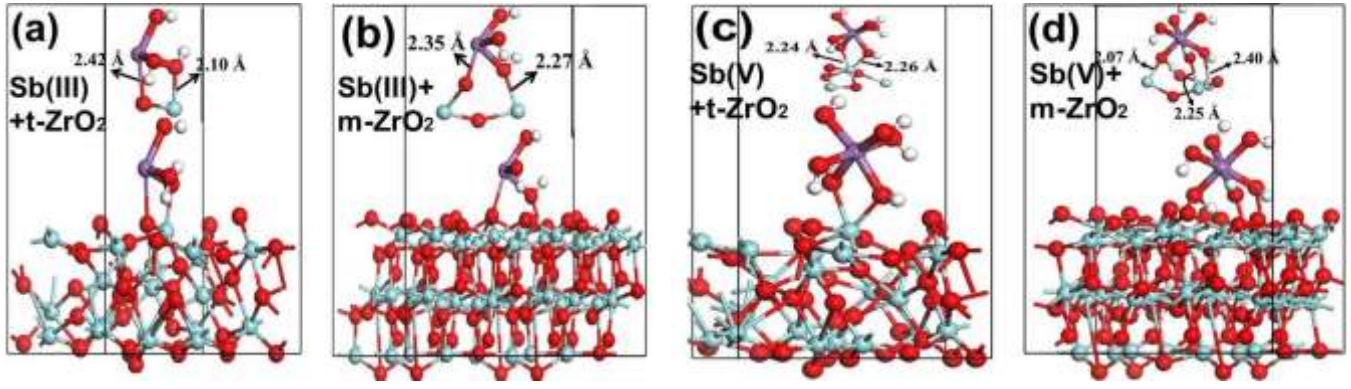
Antimony Adsorption on Novel Carbon Nanofibers Decorated with ZrO_2 (ZCN)





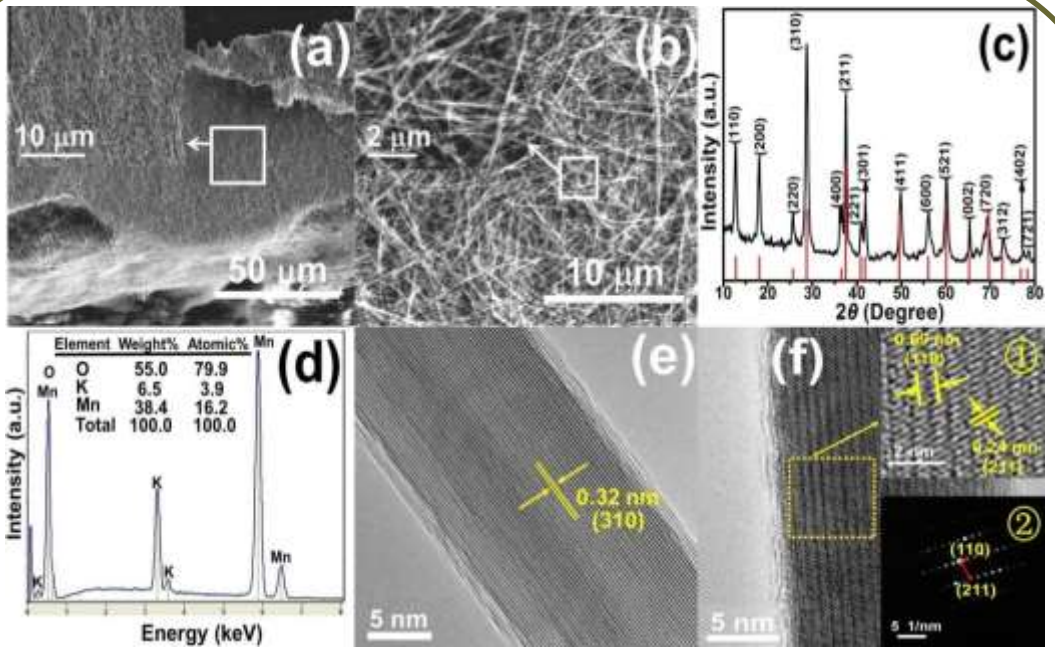
- The adsorption capacity of ZCN toward Sb(III) and Sb(V) are **70.83mg/g** and **57.17 mg/g**, respectively. And the **tetragonal ZrO_2 (t-ZrO_2)** and **monoclinic ZrO_2 (m-ZrO_2)** are coexist on ZCN. Meanwhile, the adsorption process of Sb on ZCN is determined to be **exothermic reaction**.
- **DFT calculations** revealed that both Sb(III) and Sb(V) can form stable complexes on the surface of **t-ZrO_2** and **m-ZrO_2**, with the adsorption energy (Ead) of -1.13 eV and -0.76 eV for Sb(III) and -6.07 eV and -3.35eV for Sb(V) on **t-ZrO_2** and **m-ZrO_2**, respectively. Both are **chemisorption** based on partial density of states analysis

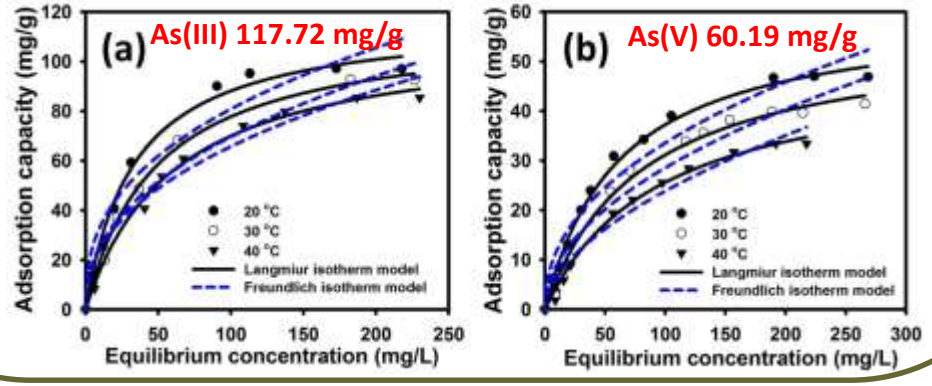
Complexes of Sb(III) and Sb(V) adsorb on different crystal form of ZrO_2

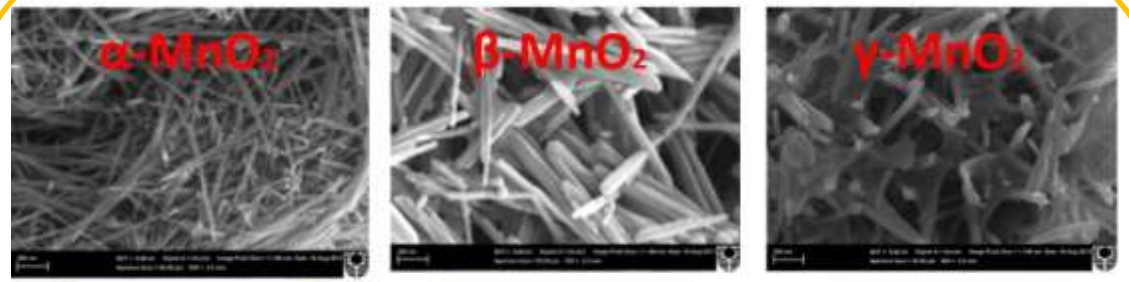


Our Work on Adsorption Process

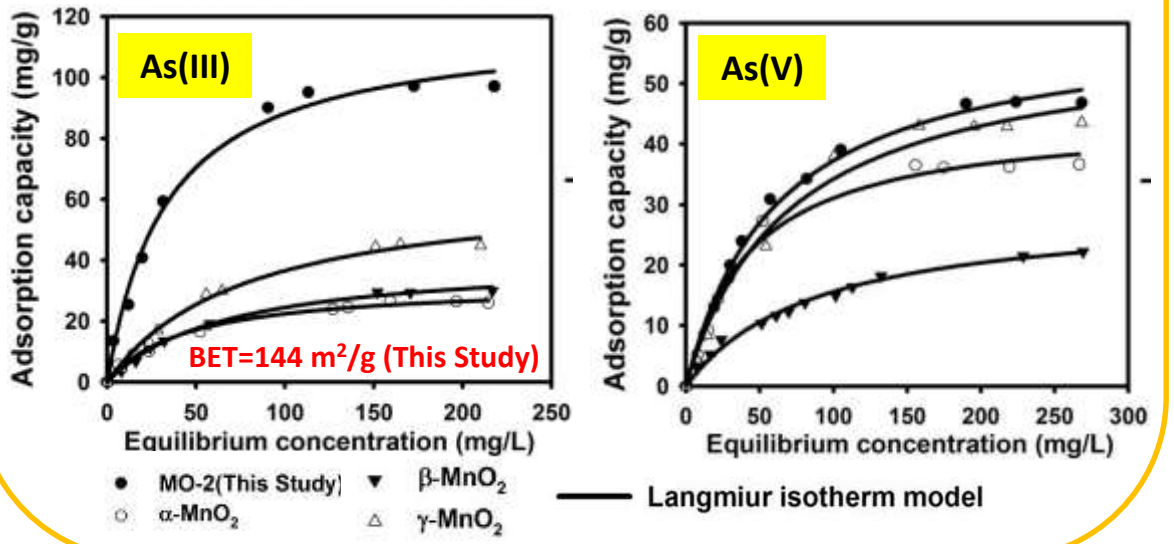
Arsenic Adsorption on Novel α-MnO_2 Nanofibers (MO-2)



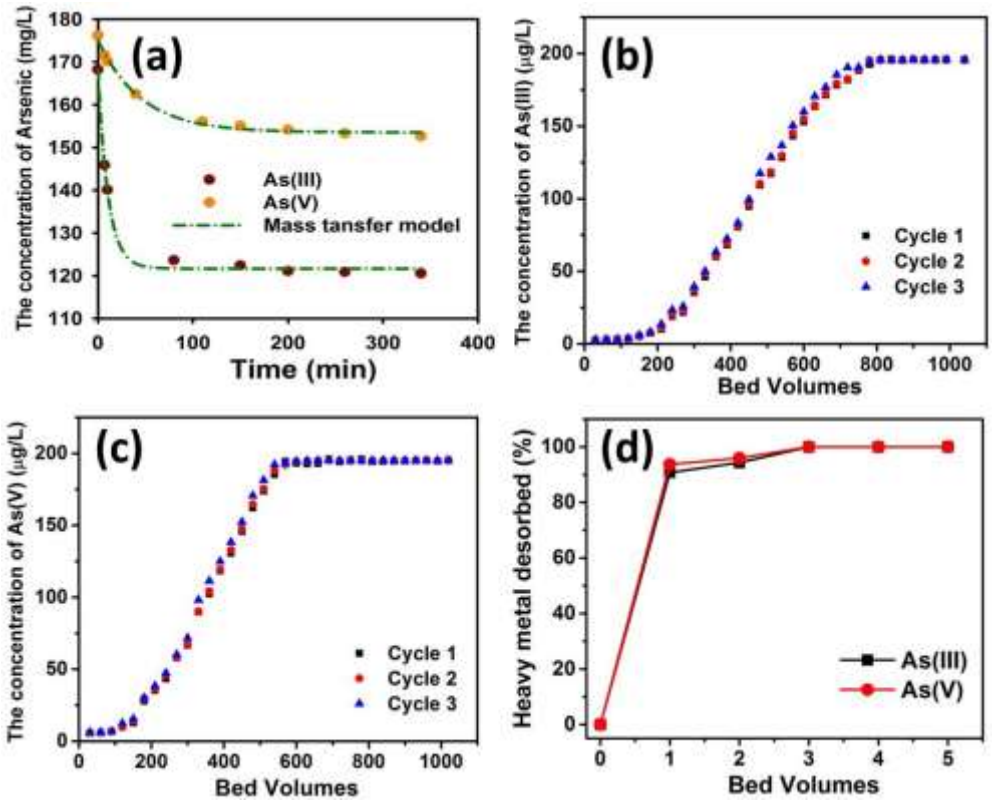




BET=148 m^2/g | BET=194 m^2/g | BET=83 m^2/g

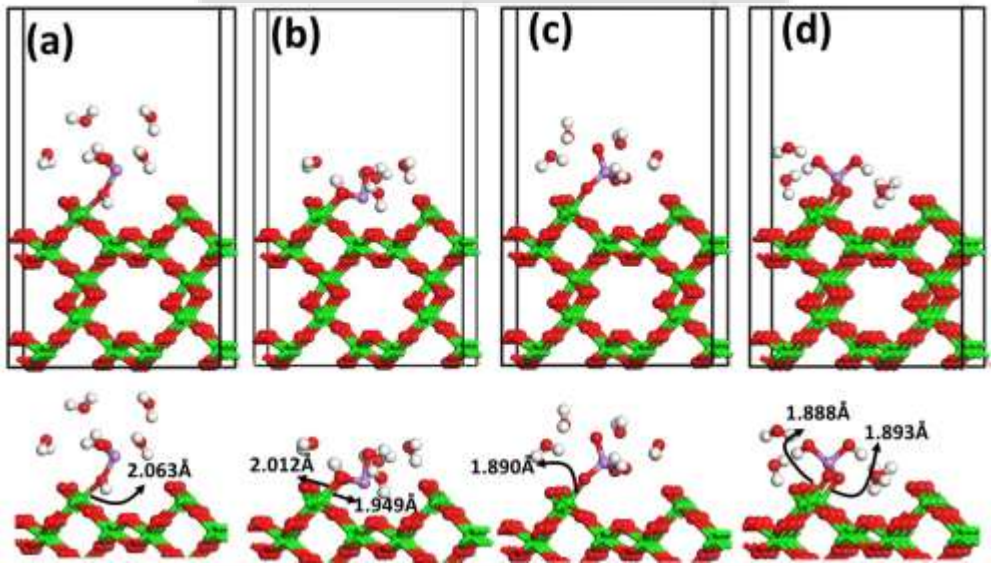


Our Work on Adsorption Process

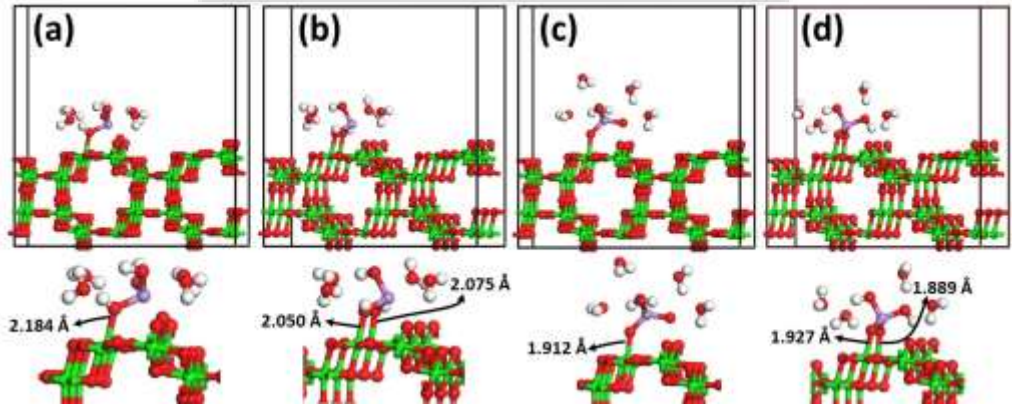


- Adsorption kinetic data was fitted with **mass transfer model**
- Fix bed column test was determined, MO-2 can treat **200 bed volumes (BV) (800 mL) for As(III)** and **120 BV (480 mL) for As(V)**, respectively, with only produce **3 BV (12 mL)** of 0.5 mol/L NaOH solution.
- DFT calculations (on the right side) unraveled that both As(III) and As(V) can **monodentate** and **bidentate** on (110) and (100), and the complexes on (100) are more stable than (110). Both are **chemisorption** based on partial density of states analysis

As(III) and As(V) adsorbed on (110)



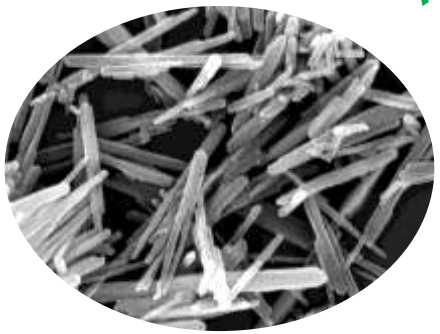
As(III) and As(V) adsorbed on (100)



Arsenic atoms are purple, oxygen atoms are red, manganese atoms are green, and hydrogen atoms are white.

Our Work on Adsorption Process

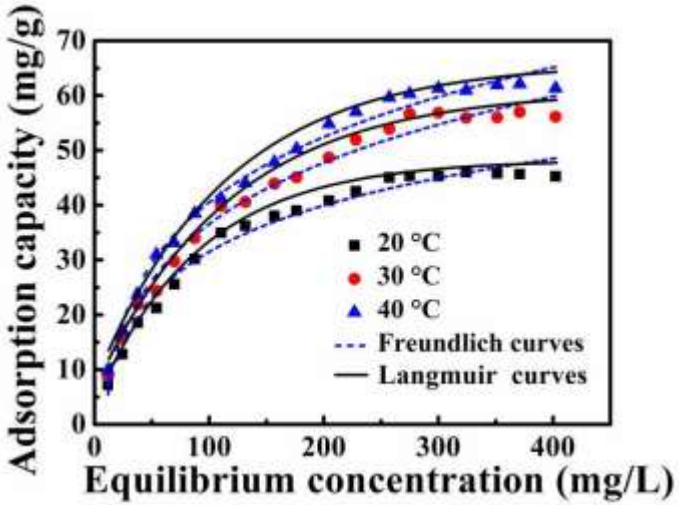
Capturing Lithium (Li) from Wastewater Using 3-D MnO_2 Ion Cages



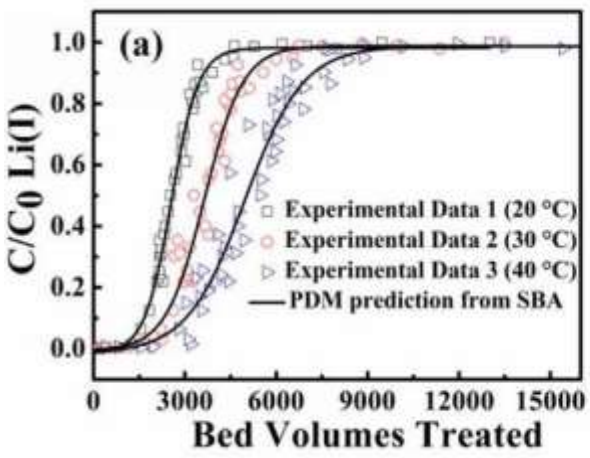
Lithium Ion Cages (CMO)

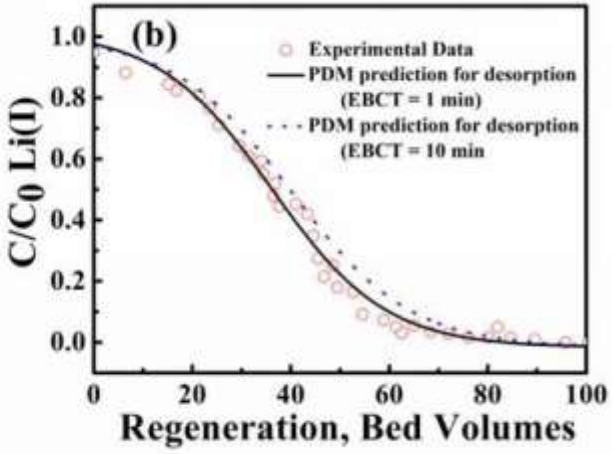
Adsorption

Prediction



- The maximum equilibrium adsorption capacity is approximately **61.32 mg/g** at equilibrium concentration about 300 mg/L at **40 ºC**, and determined to be the **endothermic reaction**.

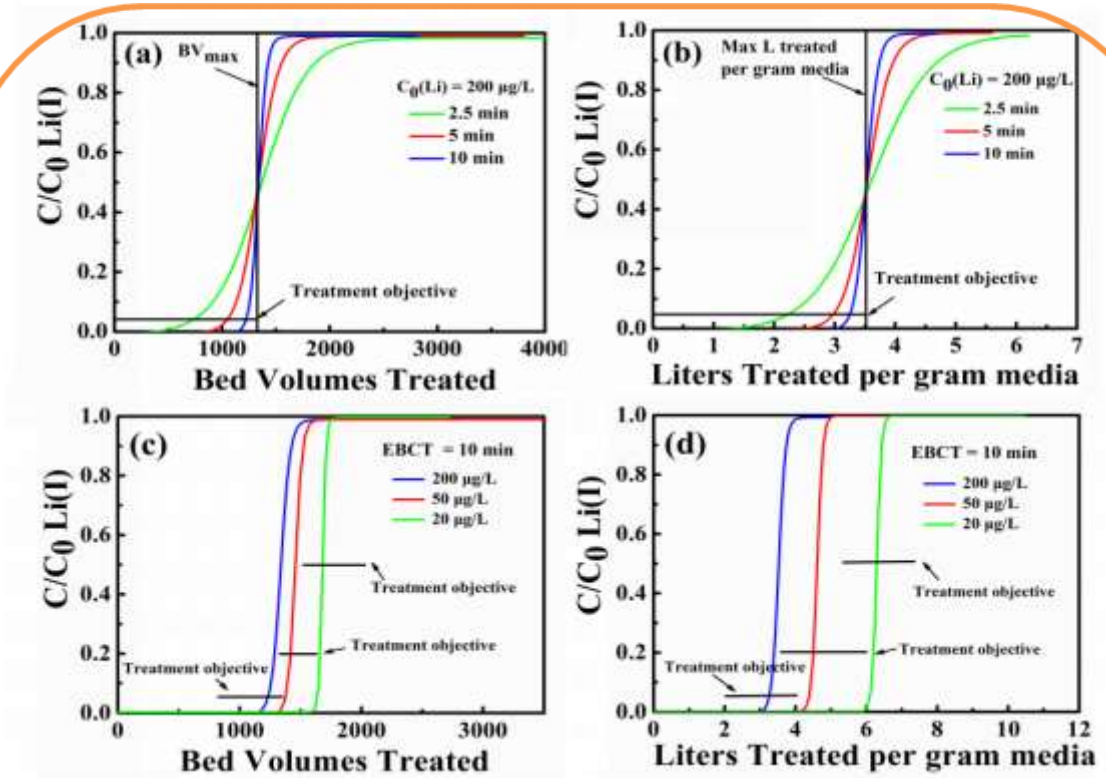




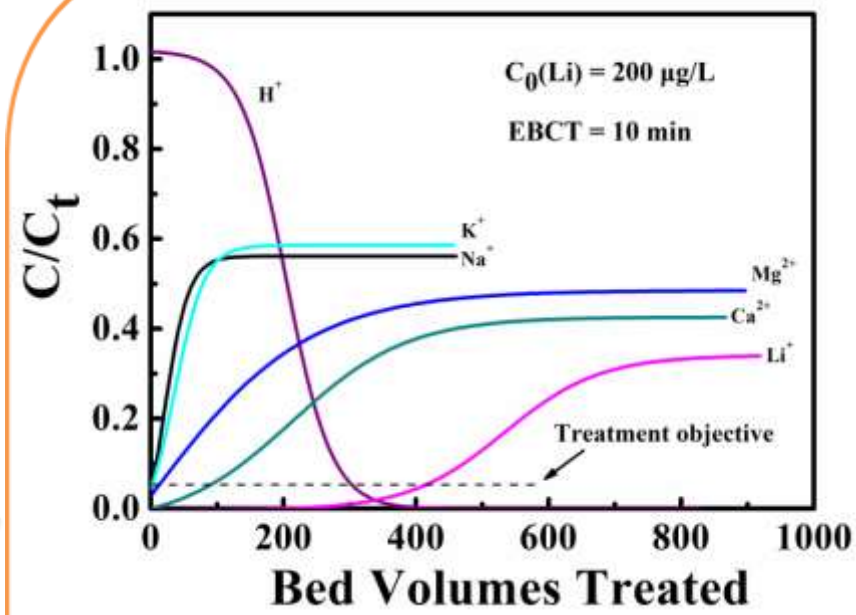
Pore Diffusion Model (PDM) Predicition for Fixed Bed

- The PDM predictions for the SBA were excellent ($R^2 \approx 0.99$). As shown in Figure 8a, in fact, the integrated capacities (areas above the curves as a function of BVs fed) were **1,374, 1972 and 2493 BVs for 20, 30 and 40 ºC**, respectively.

Our Work on Adsorption Process



- Figure a shows the full-scale breakthrough curves for EBCTs of **2.5, 5 and 10 min** and the PDM predicted that approximately **740, 1051 and 1237 BVs** can be treated, respectively. Figure b illustrates When the EBCT was **2.5, 5 and 10 min**, approximately **2.2, 2.9 and 3.2 L** of water can be treated.
- Figure c presents that when concentration increase from **20 to 200 µg/L**, BVs gradually decreased **from 1681 to 1237 BVs**, respectively. When C_0 was **20, 50 and 200 µg/L**, approximately **6.3, 4.5 and 3.2 L** of water could be treated per gram of dry media, respectively



- The other competing ions broke through earlier than Li+ which is a result of a high selectivity for Li+ over the other ions. The BVs treated when Li was by itself **1,237** for 10 minutes of EBCT and a treatment objective of 10 µg/L. This is **150, 93, 34, 4.6 times greater** (**for Na, K, Mg, Ca**, respectively) when other ions are present at concentrations that are typical in lithium ion batteries waste water.

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