

**CARBON MONOXIDE CAPTURE BY ACTIVATED COCONUT SHELL CARBON:  
TEMPERATURE-PROGRAMMED CHEMISORPTION  
AND PHYSISORPTION EXPERIMENTS**

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## **Introduction**

This project investigates the efficiency of carbon monoxide (CO) capture by activated carbon (AC) produced from coconut shell waste. Formed by incomplete combustion of carbon-based fuels, CO is a leading cause of accidental poisoning in both domestic and industrial environments worldwide<sup>1</sup>. Although commercial techniques exist for the detection and removal of CO, finding more economical alternatives using resources that are readily available in developing nations is desirable. Coconut shell waste provides an attractive alternative in this regard. Simple and scalable processes can convert this resource into AC with high potential for CO sorption. However, the mechanism of CO interaction with AC-based filters (and/or catalysts) and the factors that may control the filters' efficiency, capacity, reversibility and stability need to be clarified. It is important to know if CO captured by AC forms weak and reversible intermolecular bonds (via physisorption) and/or stronger and higher energy chemical bonds (via chemisorption). If too strong, CO sorption can become irreversible, thus preventing CO from being released back into the atmosphere. Re-adsorption and reaction phenomena during heating and cooling cycles, functionalization and humidity effects, and specific electronic interactions (e.g.,  $\pi$ -complexation in the absence of back-donating d-band electrons as in supported metals) may also aid in optimizing CO capture<sup>2,3</sup>. This study investigates these possibilities through examining CO sorption on AC by means of state-of-the-art high resolution physisorption, chemisorption and temperature programming techniques.

## **Materials and Methods**

Bio-based coconut shell waste amenable to local use in Africa was ground, digested in phosphoric acid overnight, and pyrolyzed at 800°C for 1 h to yield ~20% wt. biochar. The biochar was then re-ground and activated in CO<sub>2</sub> at 900°C for 0.25-0.75 h. For comparison, a commercial coconut shell-derived AC (YP50, Tianjin Plannano ET) was also used. Characterization of the samples via physisorption, chemisorption and temperature programming experiments was performed using instrumentation available through Penn State's Materials Characterization Lab<sup>4</sup> (MCL) via standard techniques described in detail elsewhere<sup>5</sup>.

## Results and Discussion

Gas physisorption techniques<sup>5</sup> were initially used to investigate the effects of surface pretreatments and modifications of pore structure of the AC. Isotherms, surface area and pore structure values generated for the YP50 control using MCL equipment were in excellent agreement with literature reports<sup>6</sup>. This validates the quality of the data generated for this study. More broadly, BET surface area analyses showed an increasing trend of coconut shell powder (0.94 m<sup>2</sup>/g) < biochar (919 – 967 m<sup>2</sup>/g) < activated carbon (1,701 m<sup>2</sup>/g). Activation also led to increases in the micropore area (from 700 to 826 m<sup>2</sup>/g) and t-Plot external surface area (from 233 to 874 m<sup>2</sup>/g) for the activated and non-activated samples, respectively.

CO capture uptakes reported in the literature for various commercial ACs at 298 K and 1 bar are < 10 cm<sup>3</sup>(STP)/g (or < 0.5 mmol/g)<sup>7,8</sup>. **Figure 1** compares CO uptake capacities (at 298 K and 1 bar) published in literature reports for a wide variety of adsorbents. Adsorbents towards the right hand side exceed the reported uptakes of commercial AC samples alone by a factor of 2-3. As shown in **Figure 1**, there appears to be no general correlation between CO uptakes and reported physical parameters (specific surface area, pore volumes or average pore sizes). In fact, carbon nanosheets<sup>10</sup> appear to be quite competitive with the best performing zeolites and MOFs in terms of overall CO capture. The lack of observable correlations in **Figure 1** suggests that adsorbent physical properties aid, but by themselves do not control, CO sorption. This is consistent with the complementary role that surface chemistry can play in CO capture.

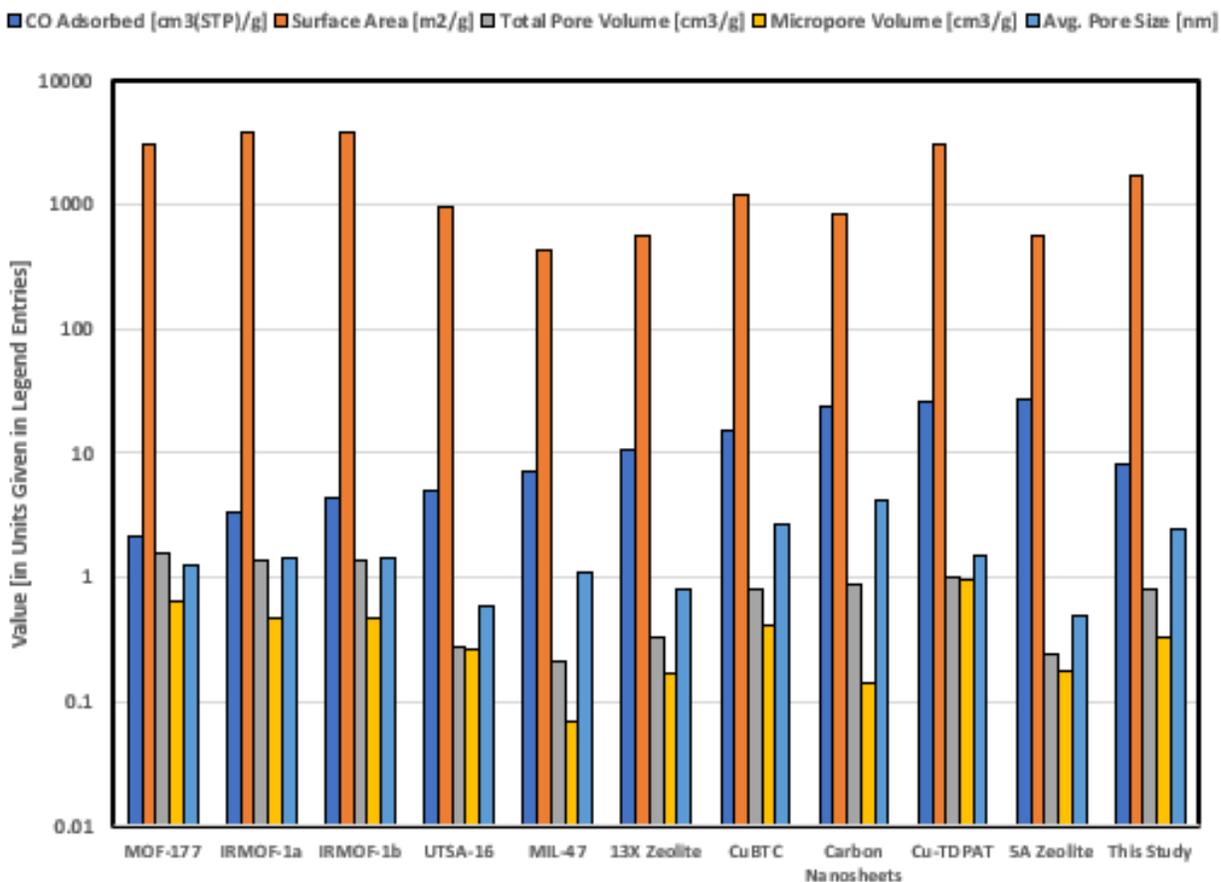


Figure 1. Comparison of CO Uptakes (298 K, 1 bar) for Adsorbents Reported Elsewhere<sup>9,10</sup> vs. This Study.

By virtue of its weak dipole moment, CO shows stronger interactions with polar or polarizable surfaces. Therefore, AC functionalization and metal salt impregnation techniques can enhance CO capture. The use of copper (I) oxide in particular has been found most useful to promote CO sorption selectivity over other gases in dynamic flow gas separation conditions. In a recent study, Li et al.<sup>11</sup> reported CO uptake capacities up to 84 cm<sup>3</sup>(STP)/g (3.75 mmol/g) at 298 K and 1 bar on a specially tailored metal-organic framework (that is, a MOF designated as MIL-100(Fe) with Cu<sup>+2</sup>-loaded cages that curtail Cu sintering during its reduction to Cu<sup>+</sup>). Copper and/or its functional analogues can also be dispersed and partially reduced if needed on AC in order to obtain the best compromise between adsorbent cost (relying on simple technologies and materials economically available in local developing regions) and CO uptake performance (particularly since AC is much more mechanically, chemically and thermally robust than MOFs). One such analogue under investigation in this study is oxidized tin, given that CO uptakes are reportedly promoted via CO-O bond formation following mild heat treatment of biochar impregnated with tin chloride.<sup>12</sup> Additional physisorption, chemisorption and temperature programming experiments are currently in progress to explore these potential pathways to optimizing CO capture.

## Conclusion

Poisonous CO can be captured using cost-effective, locally available biomass resources (such as coconut shell waste in developing regions) to produce suitable ACs. The CO uptake capacity and selectivity of AC sorbents is influenced by both their structural features and surface chemical considerations. Physisorption, chemisorption and temperature programming techniques can provide structural and chemical information necessary to assess the nature, the quantity, and the bonding quality of CO to AC-based sorbents. Knowing where, how much and how strongly CO may bond to different AC-based substrates should lead to the development of more robust, economical and practical CO capture materials than are currently available.

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