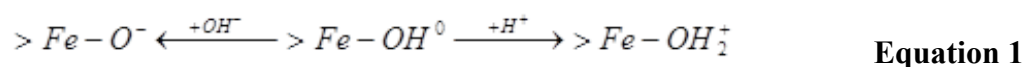


Graduate Research Plan Statement

Intellectual Merit

A novel type of adsorbent substrate based from oxidic and refractory material with high metal amphoteric oxides on its surface can be used for heavy metal removal from aqueous media. The substrate has a large active surface that can be altered by pH dependence whereby the oxides can deprotonate in alkaline medium, which increases its negative charge density and leads to favorability in cation adsorption. On the other hand, the oxides protonate in acid medium, thereby creating a positive charge density and favors anion adsorption. This scheme is outlined in equation 1 with the example of the substrate surface possessing iron oxide.



In order to do this, this substrate must be extracted from soil lacking the formation of horizons, indicating the absence of soil-forming processes pictured in figure 1. The sun dehydrates the oxides at the surface of the soil, making them irreversibly hard and ultimately limiting it for agronomical use, however experimentation of these substrates for its absorbate properties can be studied to make use of them. These soils are located near Mérida City, Venezuela and are prepared and treated in a fashion that would allow the soil-turned-substrates to be used heavy metal adsorption. A collaboration with University of Los Andes, Mérida, Venezuela would be needed to have access to the treated substrates¹.



Figure 1. Soil of interest located in Mérida City, Venezuela that once prepared

Once the raw soil has been processed, the substrate can be reacted with HCl or NaOH to produce an active surface. Running the structure of the entire substrate and its active surface in GaussView can provide more information about the atomic charges after the pH alteration, location of electron density, and type of interaction between the surface and the acid or base. For example, HCl activation of the surface should produce $Fe-OH_2^+$ substrate surface, which can be analyzed and give more contextual data about the decrease in electron density. This dissection of the pH activated surface can reveal more about the properties that favor ion adsorption, which can be expanded to apply to other surfaces to see if charge manipulation can be mirrored in other methods.

One realm of study is using the activated substrates for the study of arsenic adsorption from aqueous media. When the substrate is acid-activated, it favors anion adsorption, such as that of H_2AsO_4^- . Through adsorption and kinetics study, we can expose the activated surface with a known concentration of arsenic solution for a certain set period of time (ranging from less than an hour all the way up to 24 hours) and measure the remaining arsenic solution left in solution through the use of OES-ICP. The arsenic concentration absorbed can be found from the difference in starting concentration and remaining concentration and through fitting to a Freundlich fitting linear model, the adsorption capacity and other parameters can be calculated.

Additionally, the predicted IR spectra of the reaction between the non-activated surface (Fe-OH) and the cation/anion can be compared to the activated surface with the cation/anion for comparison of the presence of additional peaks, signifying additional interactions between the activated substrate and the ions, as well as changes in the intensity of peaks. The analysis of the thermodynamic parameters available through GaussView, ΔE , ΔS , and ΔG , can also reveal more about the favorability of the activated substrate reaction.

Broader Impacts

The application of these substrates targets the adsorption process of water filtration that other media lack. The use of these substrates for water filtration is not only cost-efficient, readily accessible, but also environmentally friendly since the substrates stem from a source that is limited in agronomical use. Through testing on the small scale, it can provide a quick visualization of the larger scale repercussions if performed on a scale many times greater.

It is particularly important to delve into arsenic adsorption since arsenic is carcinogenic and very toxic to humans, especially when consumed. The effects of prolonged arsenic exposure include the onset of genetic mutations, hinderance of cognitive development, along with plethora of abnormalities in bodily functions and systems such as reproductive, respiratory, and nervous systems. The most important precaution to take against arsenic exposure is to monitor the water supply as it is a very common means of contact with humans through the water drink or the water we use for irrigation. However, ironically it is reported that at least 140 million individuals have been consuming water above the acceptable arsenic levels of $10\text{ }\mu\text{g/L}$, coupled with alarmingly high levels of arsenic found naturally in ground water of many countries make arsenic detection and filtration an imperative point of study². The outreach and repercussions of such a project could be applicable to the removal of many other heavy metals prevalent in water such as lead, mercury, and copper that poses adverse effects in humans. Just as important, it can also provide a method of water filtration to those areas and those individuals who do not have the means to do so.

References (Times New Roman, 10-pt., single-spaced; you can remove this text)

1. Millán, Fernando & Zerpa, David & Prato, Jose & Senila, Marin & Levei, Erika-Andrea & Tănăselia, Claudiu. (2016). CHEMICAL AND PHYSICAL CHARACTERIZATION OF THREE GRANULOMETRIC FRACTIONS FROM THREE OXIDIC LITHOLOGICAL MATERIALS. 10.13140/RG.2.1.3833.6248.
2. World Health Organization. "Arsenic in Drinking Water." *WHO*, 2011, www.who.int/water_sanitation_health/dwq/chemicals/arsenic.pdf.