**OBJECTIVE AND SIGNIFICANCE:** The objective of this project is the design, synthesis, and characterization of novel, reversible high-performance acidic gas (SO\(_x\), NO\(_x\), and H\(_2\)S) contaminant absorbent materials. The materials under development will enable fuel cell vehicles to be efficiently operated under harsh atmospheric air environments. If successful, sorbents under development will assist the fuel cell filter industry, and reduce environmental contamination from hazardous absorbent waste.

**BACKGROUND:** Current state-of-the-art gas purification technologies for acidic gas capture based on metal oxides and hydroxides do not meet all of the performance requirements of today’s gas purification in terms of sorption: kinetics, capacities, selectivity, and reversibility. This leads to large volumes of polluted absorbent waste. This situation can be expected to worsen in the future with the increased use of fuel cell vehicles that require abundant efficiently purified air as an oxygen source.

The sorbent classes under development include ionic liquids, metallo ionic liquids, and MOF-activated carbons. The sorbent material properties are optimized through a combination of careful selection of reactants and modification of the sorbent cation and anion groups. For instance, metallo ionic liquids with a high content of the small, highly charged acetate and croconate groups, and transition metal ions with expandable coordinative environments are being designed, synthesized, and characterized.

Nano confinement of the absorbents in highly porous materials is being performed in order to increase acidic gas-sorbent interactions and hence gas sorption performance. Nano confinement is especially critical for ionic liquids absorbents since they have high viscosity, which limits gas diffusion distances into the bulk of the material. We have physically deposited thin films of 1-ethyl-3-methyl imidazolium acetate ionic liquid onto activated carbon that remain intact during exposure to SO\(_2\) and/or NO\(_2\) contaminated air streams. The sorbents being developed also have relevance in other applications requiring acidic gas (SO\(_x\), NO\(_x\), and H\(_2\)S) contaminant mitigation, including flue gas cleaning and natural gas purification.

**PROJECT STATUS/RESULTS:** Our work has shown that nano confined acetate based ionic liquids have high potential for SO\(_2\) capture, with higher breakthrough capacities and times observed with the 1-ethyl-3-methylimidazolium acetate, compared to pure activated carbon and activated carbon supported potassium hydroxide sorbents (Figure 1, below).

Furthermore, we have recently prepared novel acetate based metallo ionic liquids and ionic salts containing Mn and Fe with potential for acid gas capture at comparatively low cost compared to the pure ionic liquids. We have obtained the crystal structures of the anhydrous and hydrated M\(_5\)(OAc)\(_{10}\)C\(_2\)mim\(_2\) (M=Mn or Fe). Preliminary gas sorption analyses on the Fe\(_4\)(OAc)\(_{10}\)C\(_2\)mim\(_2\) sorbent indicate plausibility for reversible acid gas capture (Figure 2).

The following peer reviewed publications have resulted from this project:

• 2018, G. Severa, J. Head, K. Bethune, S. Higgins, A. Fujise, *Comparative studies of low concentration SO₂ and NO₂ sorption by activated carbon supported [C₃mim][Ac] and KOH sorbents*, Journal of Environmental Chemical Engineering, Vol. 6, Issue 1, pp. 718-727.


Figure 2. EDS analyses of Fe₄(OAc)₁₀[C₃mim]₂ material (a) as synthesized (b) after SO₂ absorption, showing intense presents of sulfur peaks (c) after SO₂ desorption at 90 °C, showing minute presence of sulfur species.

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*Contact*: Godwin Severa, severa@hawaii.edu

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