EXPLORING THE EFFICACY OF IRON DOPING IN GALLIUM (III) OXIDE AS AN ANODE IN CONVERSION-TYPE RECHARGEABLE BATTERIES.

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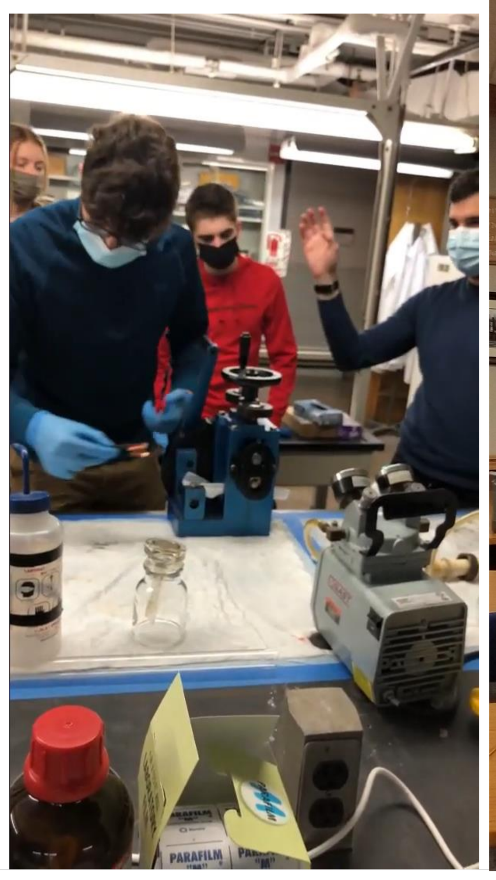
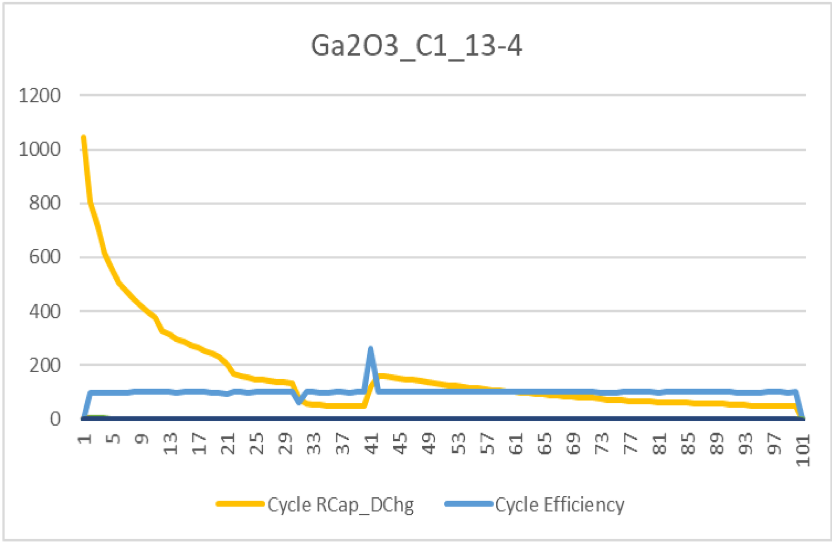
Motivation

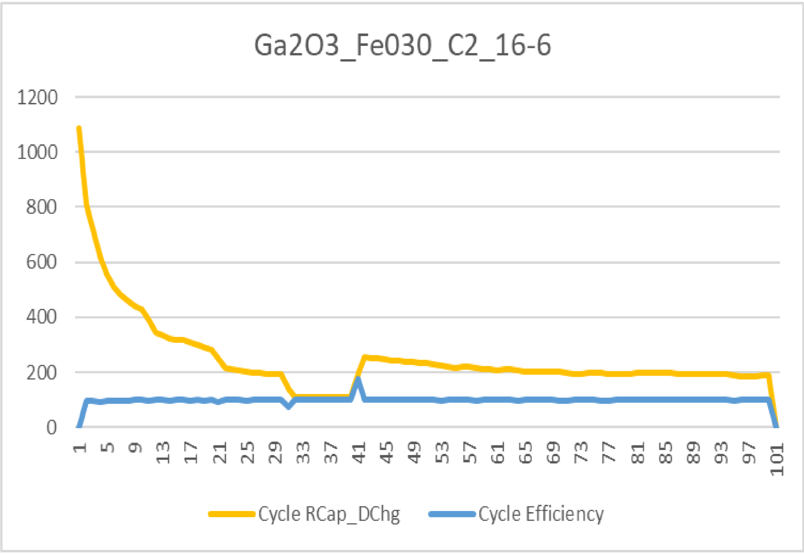
- The demand for rechargeable batteries is higher than ever, especially with the increasing popularity of portable mobile devices, personal computers, and electric vehicles. At the same time, the requirement for rechargeable batteries to be cheaper, longer-lasting, and energy-efficient for commercial use has increased. Despite their abundance in the field of electronics, the limited capacity and energy density of intercalation-type batteries display the growing need for further developments in anode and cathode materials. Conversion- type materials present a novel and promising alternative as their transformative properties have potential to increase both specific capacity and energy density. Gallium-based anodes have so far been presented as a potential solution. In recent research, gallium-based anodes have had promising results in terms of longevity and consistent energy outputs. Both gallium's self-healing properties and negative reduction potential contribute to potentially elevated specific capacity and battery cycling efficiency as an anode material. In addition, iron (Fe) doping was introduced to the material in an attempt to stabilize the structure and increase entropy. In an off-centered position, the smaller iron molecule has more atomic space to react with neighboring molecules.



Major Accomplishments

- Performed ball-milling to synthesize Gallium (III) Oxide (Ga2O3) powder
- Annealed powder to effectively dope iron into gallium oxide structure
- Performed X-Ray Diffraction (XRD) and software analysis to confirm iron doping
- Synthesized slurry with active material, carbon black, and NMP binder
- Coated slurry on copper to form half-cell electrode
- Assembled coin half cells in argon gas chamber
- Cycled batteries for 1000 hours
- Performed Extended X-Ray Absorption Fine Structure (EXAFS) at sector 10-BM at the Advanced Photon Source (APS)





Figures 1 and 2- specific capacity vs cycles for pure Ga2O3 and 0.3 mol Iron- Capacities decreased sharply as cycles increased. Iron doped sample was slightly higher.

Figure 3- Fourier Transform on Fe-doped samples and Fe foil- as cycling continues, samples resemble Fe foil, indicating nanoparticle presence

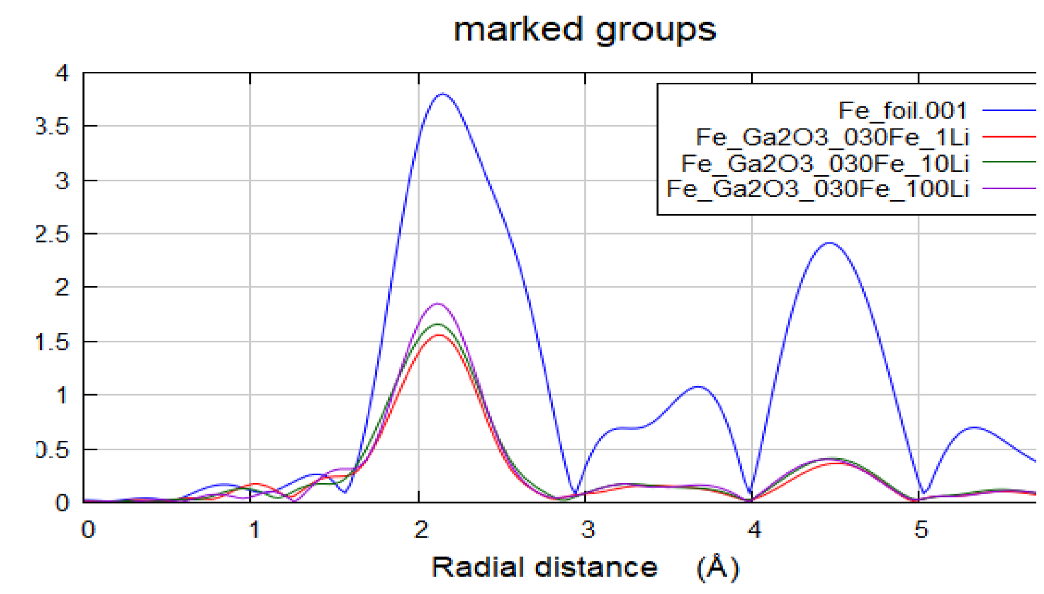


Figure 4- Fourier transform after 100 cycles of both lithiated and delithitated samples of FeGa2O3 and Ga2O3

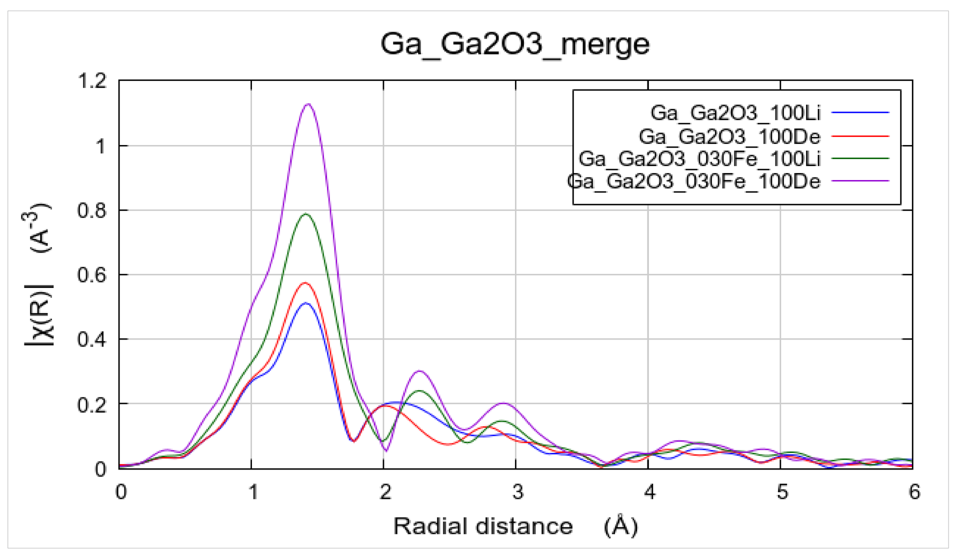
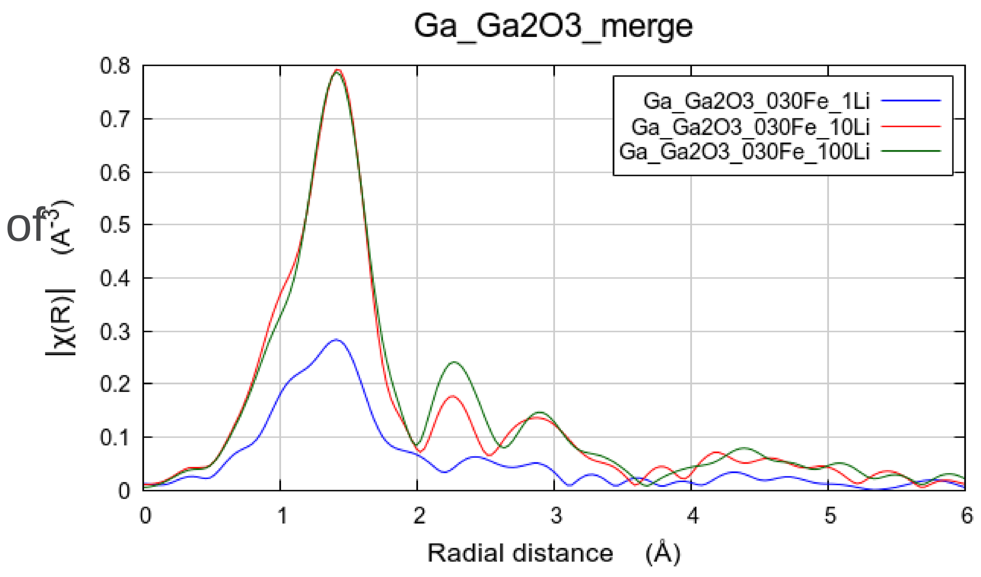


Figure 5- Fourier transform of lithiated FeGa2O3 shows most of the gallium remains oxidized while the rest breaks down into nanoparticles



Impact

- In both samples, specific capacity vs. cycles shows a sharp decline followed by a steady curve after 41 cycles
- Fourier Transform of FeGa2O3 samples and Fe foil show development of conductive Fe nanoparticles
- Between 1 and 10 lithiations of FeGa2O3, the Ga2O3 crystal structure failed and re-formed into an amorphous matrix of Ga2O3, where the produced Fe nanoparticles are suspended
- Fourier transform shows most of the Ga in the FeGa2O3 samples remains oxidized, while the remaining gallium forms Ga nanoparticles which migrate toward the Fe nanoparticle sites
- In the Ga2O3 samples, a metallic Ga-Li alloy is formed, which prevents delithiation and reduces capacity
- The continuous changes in the 100-cycle Fourier transform show that gallium participates in energy storage in the iron-doped samples, ultimately increasing specific capacity

Future Directions

- While the Ga2O3 structure failed, Fe-doping increased specific capacity
- Formation of high surface area Fe nanoparticles increased anode conductivity and show the benefits of iron doping
- Further doping mechanisms can be explored regarding molar ratios or alternative transition metals to optimize its effects
- An In-situ or operando experiment could be performed to further understand the mechanism of lithiation and delithiation in conversion- type materials

References:

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