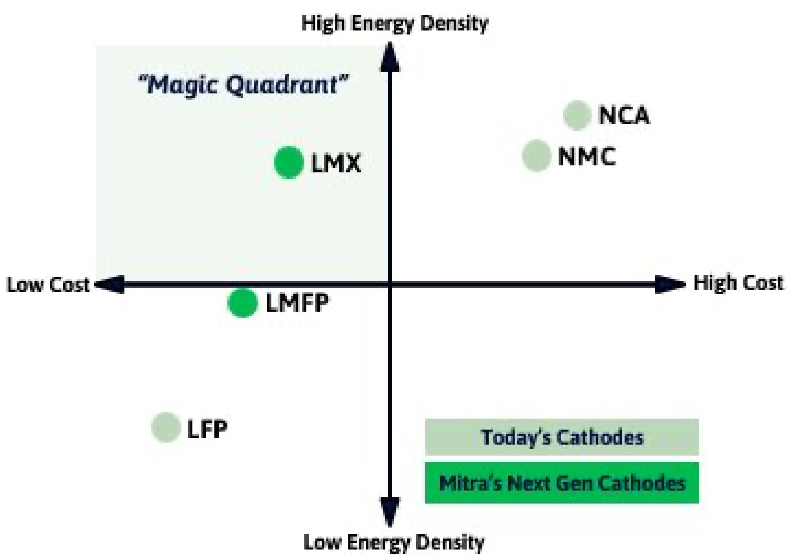
Background

Mitra Chem is a Silicon Valley startup, innovating and commercializing cathode materials to enable mass-market electrification in transportation and energy storage. Mitra Chem's first product categories focus on iron-based cathodes, specifically lithium iron phosphate (LFP) and its variant lithium manganese iron phosphate (LMFP). These iron-based cathodes shift away from incumbent NCA and NMC technologies, which are more expensive, less safe, and utilize elements such as nickel and cobalt which are facing imminent supply crunches. However, LFP and LMFP have lower energy density compared to nickel and cobalt based materials. To close this gap, the company is actively working on the development of next-generation materials (LMX) that maintain the safety and price point of LFP and LMFP but have energy densities approaching those of NMC and NCA without using Ni or Co (shown by the "Magic Quadrant" in the figure below).



Hackathon Challenge

A key differentiator for Mitra Chem is its "Atoms-to-Tons" Acceleration Platform, tailor made for cathode development. The platform combines AI, physics-based models, automation, and high-throughput experimentation to address key bottlenecks in materials research, development, and scale up. To add to our Acceleration Platform, our team is currently considering the use of Generative AI, particularly large language models (LLMs), to accelerate the discovery and development of materials that might fall in the Magic Quadrant.

Our challenge for you is to evaluate and/or demonstrate the use of generative AI to address <u>ONE</u> key bottleneck in the development of breakthrough cathodes. The potential of LLMs is immense, and there are a number of potential bottlenecks you could select from. We list a (non-exhaustive) set of ideas below for your consideration:

- **Market and Supply Chain Analysis:**
    - How can LLMs help identify scalable, sustainable, and supply chain-resilient raw materials for cathodes? How can they gather data on the availability and pricing of these materials and find potential suppliers?
    - How can LLMs quickly alert and adapt to emerging trends and/or disruptions in market conditions? Can they suggest alternative materials or sources to mitigate supply chain risks? How can LLMs assist in forecasting future market conditions and demand by analyzing data from various sources?
- **Acceleration of Materials Discovery:**
    - How can LLMs be used to mine the scientific literature or materials databases to discover new materials formulations (i.e. chemical composition and atomic structure) that may fall in the magic quadrant? Other requirements to consider here are materials synthesizability and electrochemical stability during charge-discharge cycles.
    - How can LLMs be used to develop predictive models that establish connections between materials properties and performance?
- **AI Experimental Assistant:**
    - How can LLMs be used to efficiently review and summarize the scientific and/or patent literature related to cathode materials? How can they assist researchers with natural language Q&A, ensuring appropriate citations of references?
    - How can LLMs serve as guides and optimization tools for experimental researchers performing cathode material synthesis? For example, can LLMs be used to suggest possible synthesis recipes and process conditions (e.g reaction temperature) for synthesis?

As you evaluate LLMs for your chosen focus area, it may be helpful to highlight what may be possible with state-of-the-art LLMs of today, potential shortcomings, and areas for improvement. It may also be useful to consider how to combine insights with those from additional data sources (for example, structured data in materials databases such as the Materials Project). We encourage you to include demos of how you may have used LLMs in your response, but these are not mandatory.