Materials Informatics: Predictive Modeling for Crystal Structure in Lithium-ion Battery Cathode Materials

Group Members: Hao Wang (2344601), Udom Ifeanyi (2220031), Kevin Tieu (1902070)

Background:
Lithium-ion battery cathode materials are critical for facilitating the de-intercalation of lithium ions within batteries. The crystal structure is pivotal in understanding lithium-ion battery performance. The unique characteristics of their crystal structures significantly influence the efficacy of lithium-ion de-intercalation, ultimately impacting the electrochemical performance of these batteries. This study aims to investigate possible correlations between various chemical and physical properties in order to predict crystal structures using state-of-the-art machine learning models.

Dataset:

- **Source:** Crystal System Properties for Li-ion batteries dataset provide data about the physical and chemical properties of several Li-ion silicate cathodes.
- **Data points:** The dataset contains 339 data points (samples). There is no missing or mismatched data points.
- **Features:** The dataset has 8 features: Space group, formation energy, energy above hull, band gap, number of sites (Nsites), density, volume, band structure, elemental composition (e.g., Li, Mn, Si, O, Fe, Co)
- **Learning Target:** Crystal structure of lithium-ion battery's cathode materials. The crystal structure has three classes: monoclinic, orthorhombic and triclinic.

Plan of Work:

1. **Data Preprocessing:** The chemparse library is used to extract the stoichiometry of elements in the cathode materials from their chemical formulas. Then, these supplementary data are combined with the main data set to provide a richer and more informative feature set.
2. **Data Analysis:** The initial phase of data analysis involved the generation of a heatmap, providing a holistic view of the dataset. This heatmap revealed potential correlations among different properties, serving as the foundation for further investigation.
3. **Classification Task:** The Gradient Boosting algorithm will be used as the training model to predict the crystal structure of the cathode materials based on their properties and composition.
4. **Model Evaluation:** For each machine learning iteration, the model will be evaluated using appropriate metrics to measure its accuracy and precision.

References:

1. D. Agarwal, "Crystal System Properties for Li-ion batteries," Kaggle, 2023. [Online]. Available: https://www.kaggle.com/datasets/divyansh22/crystal-system-properties-for-liion-batteries/

2. "Seaborn Heatmap: A Comprehensive Guide," [Online]. Available: https://www.geeksforgeeks.org/seaborn-heatmap-a-comprehensive-guide/. [Accessed: 19-10-2023].