**Socratic Prompting with Argo: Assessment**

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**Original Prompt:**

“What is the role of SEI/CEI in Lithium-ion batteries?”

**Socratic Reformulation:**

How can we define the roles of the Solid Electrolyte Interphase (SEI) and Cathode Electrolyte Interphase (CEI) in Lithium-ion batteries, considering the irony that while they are essential for battery operation, they can also detrimentally affect performance? How do differing perspectives on their dual nature contribute to our understanding of battery technology?

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| **Principles** | **(Follow-Up) Prompts** |
|  | **Original Prompt:**  How can we define the roles of the Solid Electrolyte Interphase (SEI) and Cathode Electrolyte Interphase (CEI) in Lithium-ion batteries, considering the irony that while they are essential for battery operation, they can also detrimentally affect performance? How do differing perspectives on their dual nature contribute to our understanding of battery technology? |
| **Dialectic** | **Follow-up Prompt 1:**  How do differing scientific perspectives on the mechanisms of SEI and CEI formation contribute to a more comprehensive definition of their roles in Lithium-ion batteries? What are the implications of these roles for future battery technology advancements? |
| **Hypothesis Elimination:** | **Follow-up Prompt 2:**  “What are the competing hypotheses regarding the formation and stability of SEI and CEI, and how can we test these to determine the most accurate explanations?” |
| **Elenchus** | **Follow-up Prompt 3:**  “Are there any assumptions about the effectiveness of SEI and CEI that might be challenged by recent research findings? How do these assumptions hold up under scrutiny? |
| **Dialectic** | **Follow-up Prompt 4:**  How do differing scientific perspectives on the mechanisms of SEI and CEI formation contribute to a more comprehensive definition of their roles in Lithium-ion batteries? What are the implications of these roles for future battery technology advancements? |

1. **Motivation**

*Why is this problem important in chemistry/materials science?*

SEI and CEI are decomposition products that cover the surface of anode (SEI) and cathode (CEI) electrode surfaces in Li-ion batteries. In their absence, reactive electrode surfaces continue to engage in side reactions with electrolyte, leading to consumption of both the electrolyte and active materials, thereby degrading the health of the battery. The SEI and CEI are intentionally formed through “formation cycles” during the initial operation of the battery, in hopes of creating a thin, ionically conductive, passivating and stable layer between the active material surfaces and the electrolyte to limit the side reactions between them.

While these layers are critical in limiting the side reactions, they also are the primary reason behind the impedance growth and cell failure, as they continue to grow during electrochemical cycling and perpetually consume the active materials and electrolyte.

It’s a critical mission to control the chemical composition, mechanical and physical properties of the SEI/CEI layers in Li-ion batteries, in order to extend their lifetime and safety.

*What challenges exist in solving this problem using traditional LLM approaches?*

The textbook definition of these systems fails to capture their complexity and dual nature. The initial direct assessment paints a picture of a uniform, static and stable structure (layer) that serves as a barrier between the active surfaces and the electrolyte. In reality, the decomposition products (SEI/CEI) are non-uniform, possess a complex chemical and physical distribution across the active layers, dynamically and continually form during aging and cycling of the battery and can manifest in both positive and negative outcomes for the cell, depending on its chemistry, mechanics and evolution.

*How could a structured Socratic approach improve reasoning and outcomes?*

The Socratic approach tackles the one-sided notions on the SEI/CEI formation in LIBs, which largely misses the real nature of these structures.

1. **What Are the Prompts Used?**

***Original Prompt:***

“What is the role of SEI/CEI in Lithium-ion batteries?”

***Socratic Reformulation:***

How can we define the roles of the Solid Electrolyte Interphase (SEI) and Cathode Electrolyte Interphase (CEI) in Lithium-ion batteries, considering the irony that while they are essential for battery operation, they can also detrimentally affect performance? How do differing perspectives on their dual nature contribute to our understanding of battery technology?

1. **What Are the Outcomes of This Example?**

*How did the LLM refine its answers over iterations?*

The direct question fails to account for the dual nature of SEI/CEI, it only captures the benefits of SEI such as stabilization and improved efficiency. With Socratic approach, it was able to generate questions that could tackle the dual positive and negative nature of the SEI/CEI in stability of LIBs. The follow up questions generated by the Socratic prompt lead to more discussion on criticality of chemical composition, mechanical properties and necessity for characterization of these layers and the various methods scientists use to maximize the benefit of these layers and suppress overgrowth which leads to lifetime decay.

*What key insights or discoveries emerged?*

The competing hypothesis method highlights the fact that there isn’t a conclusive single understanding of the properties of the SEI/CEI layers, this is a subject that’s still under investigation which gains new perspectives with emerging characterization methods that helps shed a better light to the link between its function and properties.

Few highlights from the answers:

“Research indicates that thinner, well-formed SEI and CEI can provide sufficient protection while minimizing resistance. This has led to a focus on optimizing the quality rather than the thickness of these layers.”

“In-situ and operando studies have shown that the SEI and CEI can undergo continuous changes, affecting their composition and structure. This dynamic nature can lead to increased resistance and capacity fade, challenging the notion of their static stability.”

*Any unexpected results or challenges?*

Not found

1. **Comparison to a Non-Socratic Approach**

*How did reasoning depth, self-correction, and hypothesis refinement compare?*

The non-socratic method provides foundational understanding of how SEI and CEI impact battery longevity and performance, giving a concise picture of current research without delving into deeper, emerging scientific debates. Initially, with “what is the role of SEI prompt” provides only the positive impact of these layers for both methods, and both methods miss the dual nature of the formation of these layers. They both describe it as a static, non-changing during the aging or cycling of the battery, which we know are incorrect assumptions. The Socratic prompts were capable of challenging these insufficient descriptions about the SEI/CEI layer and provide a more accurate description of their role in the cell – one that has dual implications. While these layers can provide stability when carefully formulated and formed, they also are not static, and continue to evolve during the lifetime of the battery and have very complex chemical and physical properties that we are still understanding how to optimize.

Competing hypothesis method identifies specific advanced characterization methods (XPS, TEM, EIS etc.) we utilize to test specific hypotheses we have on composition-structure-function relationships in SEI/CEI layers in batteries. Depending on the chemistry, mechanical and physical properties of the SEI/CEI layers, they can be detrimental or beneficial to the battery’s lifetime.

Regular Prompting delivers direct, factual, and scientifically accurate information that is easy to digest.

Socratic Prompting builds a framework for deep, iterative exploration, encouraging users to think critically and challenge existing assumptions, which can lead to a more refined and evolving understanding of the topic. Able to provide nuance, rather than generally accepted statements.

*Would a traditional direct-answer prompt have produced different results?*

Traditional approach gives only general responses, and fails to address the nuances of dual nature of these SEI/CEI layers.

*Did the Socratic method improve clarity, adaptability, or accuracy?*

Overall, I am satisfied with the response of Socratic method, although when we use the socratic prompts generated by the socratic agent and input them into the regular LLM, it provided longer answers than the socratic agent. Using the socratic prompts, the LLM was able to capture the false assumptions (the continuous evolution of the SEI/CEI, importance of chemical and physical properties of the SEI/CEI in its functionality, etc.) and tackle these false assumptions by providing running hypotheses we have on the implications of SEI/CEI.