**My Assessment**

**Feb 24, 2025**

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**Motivation of the Problem**

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

Non-aqueous Zn-organic batteries have gathered attention as the next-generation batteries due to the high theoretical energy density, improved sustainability, and cost-effectiveness. However, the low Zn solubility and ion conductivity of the organic solvents limit their practical applications. Understanding Zn-binding energy of organic solvents will play a crucial role in discovering and designing better organic solvents.

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

The Zn-binding energy of a variety of organics is multi-dimensional problem that needs to be tackled considering various molecular properties and coordination chemistry. From my experience, traditional LLM tools could successfully suggest crucial aspects, e.g., the necessity of standardized metric for evaluation and the importance of the steric effects. However, they often failed at identifying the core question and suggesting solutions, potentially due to the complexity of the question itself.

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

The Socratic approach successfully identified the most important question of the given prompt, leading to significantly improved quality of response. The suggestion from the Socratic assistant is what I expected as a researcher with expertise in the field. Although ChatGPT without the Socratic prompt suggested the same solution, it was a part of many responses, most of which are not useful to me. On the other hand, the Socratic assistant brought the idea as the most promising solution. Further, the follow-up questions guided me to clarify the underlying physical phenomena that need to be understood.

• The specific sequence of Socratic principles applied (e.g., Definition → Hypothesis Elimination → Dialectic → Analogy).

• Justification for choosing this approach—link to the scientific method if possible.

**Initial prompt** (automatically selected by SM): Definition, Hypothesis Elimination, Generalization

**1st follow-up prompt** (manually selected from suggestions): Elenchus, Analogy, Induction

* The Socratic assistant’s suggestion to the initial prompt was normalization of binding energy, which is what I expected. The Elenchus principle examined the assumptions behind this idea, which helped me go deeper to clarify the limitations. I also found Analogy 🡪 Induction step helpful to see if the idea can be appropriate. Collectively, this sequence helped to see both pros and cons of the suggested idea.

**2nd follow-up prompt** (automatically selected by SM): Definition, Dialectic, Hypothesis Elimination

**3rd follow-up prompt** (manually selected from suggestions): Definition, Hypothesis Elimination, Dialectic

* In the 2nd follow-up prompt, I brought a hypothetical (but likely to happen) example that may not be appropriately addressed by the first suggestion (normalization), which led the Socratic assistant to defining another metric (unnormalized binding energy). I wanted to define two metrics more clearly, especially connecting them to the bigger picture, the solubility. The following hypothesis elimination 🡪 dialectic principles helped me take a closer look at both metrics, leading to the conclusion that both could be useful and either of them may not fully describe the phenomenon by itself.

**What Are the Prompts Used?**

• The initial user input or problem statement.

• The system reformulation into Socratic prompts.

• The follow-up questions guiding the LLM through structured reasoning.

• Indicate whether the model-generated follow-up prompts were used or if you created your own.

Check the other document “Feb24\_Argo\_Transcript.docx”.

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

• How did the LLM refine its answers over iterations?

It refined its answers very well as it goes through the couple of follow-up Q&As. However, to reach sound conclusions, I had to provide a counterexample that the Socratic assistant could not come up with.

• What key insights or discoveries emerged?

The Socratic assistant revealed an important point, especially through Hypothesis Elimination 🡪 Dialectic steps, that the description of Zn solvation in organic solvents in terms of the Zn-binding energy is not straightforward and there is a chance that both metrics (normalized vs. unnormalized) may be necessary.

• Any unexpected results or challenges?

No, there were no unexpected results or challenges.

**Comparison to a Non-Socratic Approach**

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

They were improved compared to the traditional LLM (non-Socratic) in that the non-Socratic version simply listed some ideas, some of which were useful and the others are not, whereas the Socratic version clearly identified the core problems and gave the response to them. In other words, I felt the Socratic prompt help the LLM find a hierarchy of problems, so was to improve the quality of the response by focusing on the problems with higher importance.

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

The traditional LLM did not produce different results to the initial question. Rather, its response covered a wider range of perspectives, and the response of the Socratic assistant is a part of them. It should be noted that, however, I found many bullet points that the traditional LLM provided unsatisfactory.

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

The Socratic method improved clarity for sure as discussed above. I did not have enough experience with the Socratic method, since the conversation was made within the given topic, which is very specific. In terms of the accuracy, I did not feel any improvement, since neither of them (i.e., with and without the Socratic method) provide any wrong or misleading information. This will also be clarified with more and more trials.