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| --- | --- | --- | --- |
| Participant | General Task | Socratic Task | Methods |
| Aggarwal Abhishek | YES | NO | - |
| Chiara Bissolotti | NO | YES | Definition, Recollection, Induction |
| Sengupta Bratin | YES | NO | - |
| Işıksu Büyüker | YES | YES | Definition, Induction, Hypothesis Elimination |
| Lateer Jolaoso | YES | YES | Hypothesis Elimination, Definition |
| Johnson Luke | YES | YES | There is no mention of methods |
| Michael Stuhr | YES | YES | Hypothesis Elimination, Dialectic |
| Hong Sungil | YES | YES | Definition, Hypothesis Elimination, Generalization |
| Mustafa Unal\_SiC | YES | YES | Definition, Induction, Recollection |
| Mustafa Unal\_Oxide | YES | YES | Induction, Definition, Hypothesis Elimination |
| Mustafa Unal\_CsPBBr3 | YES | YES | Hypothesis Elimination, Induction, Elenchus |
| Yunkai Sun\_YKS | YES | YES | Hypothesis Elimination, Definition, Induction |

**Brief summary and synthesis:**

1. Overview and synthesis:
   1. Four different prompting styles: general, science assistant, Socratic prompts without System prompt, Socratic prompt with the System prompt.
   2. Socratic prompt is useful for a deep dive into a specific topic. Answers are more precise and critical (instead of a general answer from the non-SM method)
   3. Socratic prompt leads to a very focused and connected conversation session. Severe diffusion was observed for non-SM method conversation sessions.
   4. Socratic prompt might have difficulty in solving the surface-level, detailed problem (e.g., finding the equation from the literature about oxidation rate).
2. AA: Free energy barriers governing water permeation into an oil phase – Need SM method prompts. Two groups of conventional methods.
   1. Overview of content:
      1. Socratic prompting style gives more comprehensive guidance on further simulations and helps the user refine the hypothesis. Novelty of the answers is not affected.
   2. Transcript:
      1. The SM one is with Socratic style question formulation, instead of SM preprompt.
3. CB: Standard Model searches be included in analyses to achieve a 3D imaging of the proton – Need conventional prompt method.
   1. Overview of content:
      1. Socratic prompts give more precise context (historical and conceptual) than the general answer from the LLM without the Socratic prompt. SM guides the hypothesis refinement of the scientific inquiry for a very domain-specific problem.
4. SB: For what reasons a zwitterion modified PVDF membrane becomes antifouling in nature? – Need SM method. Convention and Science Assistant comparison available.
   1. Overview of content
   2. Transcript:
      1. The SM one is with Socratic style question formulation, instead of SM preprompt.
      2. It’s a comparison between direct prompting vs follow-up prompts designed based on the SM philosophy, instead of the system prompt.
5. IB: Role of SEI/CEI in Lithium-ion batteries – General Assistant vs SM
   1. Overview of content:
      1. SM prompt leads to a more critical analysis of the SEI/CEI roles (both beneficial and detrimental). General assistant provides statements that are less nuanced but easier to digest.
   2. Transcript:
6. LJ: Formulation for the anode of protonic ceramic electrochemical cells – General Assistant vs incomplete SM(?)
   1. Overview of content:
      1. Socratic method provides brief and follow-up questions. Non-SM gives general and comprehensive answers.
   2. Transcript:
7. JL: MC simulation in the NPT ensemble, - Science Assistant vs SM (incomplete?)
   1. Overview of content:
   2. Transcript:
8. MS: Multi-channel thermal decomposition reactions – General Assistant vs SM
   1. Overview of content:
      1. SM method has better focus than the non-SM conversations. Using follow-up to refine the answers from the general assistant conversation is very difficult.
      2. SM method is more accurate and precise on handling in-depth discussions.
      3. SM method has better focus on the domain-specific topic than the non-SM method.
   2. Transcript:
9. HS: Binding energy of organic solvents to the Zn cation (2+) using molecular orbital DFT calculations (Gaussian). – SM (need control group)
   1. Overview of content:
      1. Socratic method is more accurate on addressing the key of the question from the user.
      2. Follow up prompt is useful for in-depth discussion.
      3. SM might help LLM find a hierarchical solution to a complex problem.
      4. Accuracy (correctness of answers) is similar between two methods.
   2. Transcript:
10. MU-1: Mechanisms that leads to degradation on the performance of CsPbBr3 radiation detectors used in X-ray and gamma-ray detection applications. - General Assistant and SM
    1. Overview of content:
       1. Non-SM prompt failed to catch the key of the user’s question. Socratic prompt gives short and accurate domain-specific answer, and caught the domain-specific nature of the question.
    2. Transcript:
11. MU-2: Calculate the oxidation rate of lead and bismuth thin films. - General Assistant and SM, with reference upload
    1. Overview of content:
       1. SM prompt failed to critically analyze the reference uploaded. The traditional method is more helpful in providing equations and calculations from the reference.
          1. SM might be a good reasoning module, instead of an analyzer. I wonder if a mixed multi-agent system can work better.
          2. SM focuses too much on the depth but fails to catch the apparent answer or detailed information from the reference.
    2. Transcript:
12. MU-3: perform dislocation density analysis on SiC wafers - General Assistant and SM
    1. Overview of content:
       1. Non-SM method has a severe diffusion problem over conversations.
       2. SM method leads to a more focused and in-depth analysis of the problem.
    2. Transcript:
13. YS: choose electrolyte system and deposition parameters for Fe-Pt electrodeposition.- Science Assistant and SM
    1. Overview of content:
       1. SM provides a more systematic and in-depth analysis. Non-SM loses focus faster than the SM method.
       2. SM method might trade depth with creativity (diffusion of ideas).
       3. SM method is less susceptible to the prompt bias from the user.
    2. Transcript: