Task prompt and transcript corresponding to the analyses summarized in Figure 1-5 in the main manuscript.

For X-ray fluorescence, the material is exposed to high-energy X-rays that knock out a core electron and then an electron from a higher energy orbital moves into that lower energy state. When that happens, a photon is released. Let's say that when the X-rays hit the ferro-gallus ink, it knocks out an electron from the $1s$ orbital and an electron from the $2p$ orbital replaces it and releases a photon. Use the diagrams below to illustrate this process.

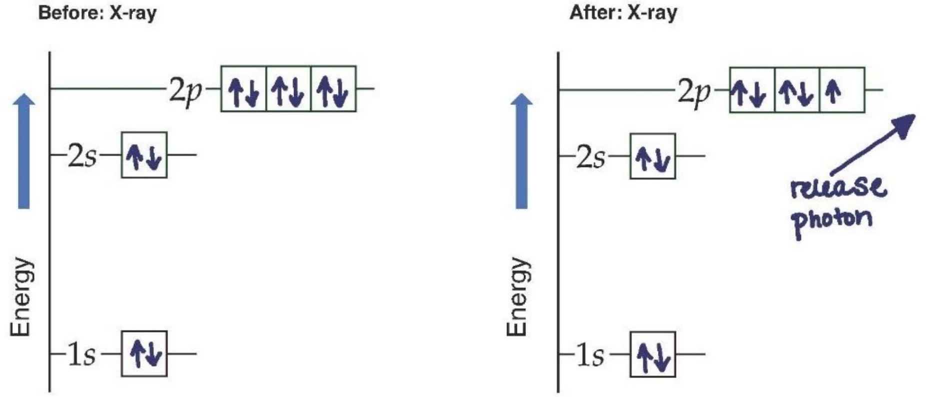


Fig. S1. Task Prompt with group work done by Shakespeare, Lewis, Evans, and Dahl

(1) Shakespeare: Basically, one electron from the 1s goes away and one of the electrons from the 2p replaces it by going down to the 1s.
(2) Lewis interrupts Shakespeare: Okay so it goes from…
(3) Shakespeare: Because you need to fill it back up
(4) Lewis: $2p^6$ to $2p^5$ to replace the…
(5) Shakespeare: To replace the 1s which has lost energy.
(6) Lewis interrupts Shakespeare: …the one that lost an electron.
(7) Shakespeare: Yup
Shakespeare: And then that process emits a photon basically.
(8) Evans: *huff*
(9) [*Lewis starts interaction with TA.Hermione about their answer to problem 5.*]
(10) Shakespeare: Ah for that ummm draw these in like you did last time.
(11) Evans: All of them?
(12) Shakespeare: Just for the first diagram.
Shakespeare: So the 1s would have two electrons, 2s would have two electrons.
(13) Evans: And then 6 here? [*Pointing at 2p orbital*]
(14) Shakespeare: Yup.
Shakespeare: And then for that one, 2s is going to be the same.
(15) Dahl: I was listening to [*TA. Hermione*]. What problem are we working on?
(16) Shakespeare directed at Evans: And then 2p is going to have five electrons instead of six, so the last one would just have one. And then 1s is going to have two.
(17) Evans: But then wouldn't it have to be…
(18) Dahl: So what question?
(19) Evans: So instead of… [*pause*]
(20) Shakespeare: It says, knock out an electron from 1s, and then put one of the electrons from 2p where that 1s electron was, so everything looks the same except this is five instead of six.
(21) Evans: What does that…
(22) Shakespeare interrupts Evans: And then you released a photon.
(23) Evans to Shakespeare: Like that? [*Pointing to what they drew and wrote.*]
(24) Dahl: Yeah
(25) Shakespeare: Photon not proton.
(26) Evans: **Giggles** [*Erases proton and changes it to photon.*]
(27) Lewis to TA.Hermione: Thank you!

Detailed application of Student Interaction Discourse Moves (SIDM) to transcript conversation from Figure 1-5 in main manuscript.

Student Interaction Discourse Moves three-tiered analytical framework (Figure 1 in (Nennig* et al.*, 2023))

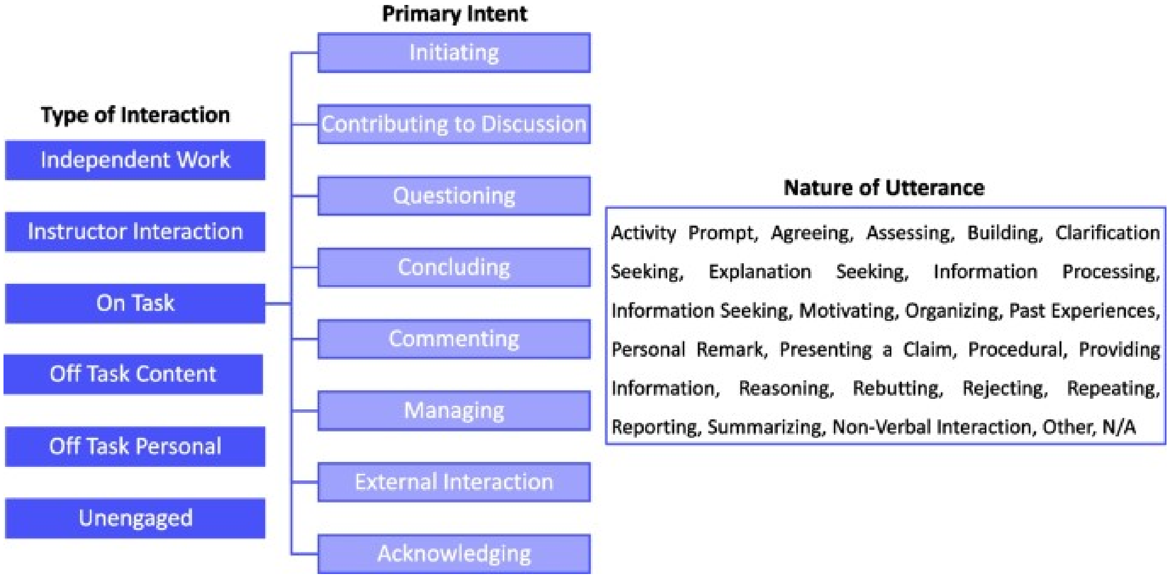


Fig. S2*. Student Interaction Discourse Moves (SIDM) graphic of three-tiered analytical framework (Fig. 1 in (Nennig* et al.*, 2023) used with permission from authors)*

SIDM Code Books. (Tables 1-3 from (Nennig et al.*, 2023))*

Table S1. *First tier of Student Interaction Discourse Moves (SIDM) Analytical Framework codes – Type of Interaction. (Table 1 in (Nennig* et al.*, 2023))*

Type of Interaction: Describes students' interactions during small group activities

Category	Definition
Independent Work (Ind W)	Students are not conversing with each other but are actively working through the problem (ex. no feedback from peers, writing stuff down, using a calculator)
Instructor Interaction (Inst I)	Interactions with the instructors about class content or administrative matters
Off-Task Content Related (Off C)	Students engaging in conversation that deviates from their assigned task but is still related to class content
Off-Task Personal (Off P)	Students engaging in conversation not related to class content (ex. personal experiences)
On Task (On)	Students are actively conversing with each other on the assigned task
Unengaged (U)	Not participating in classroom activities or engaging with peers (ex. sitting, using a phone)

***Table S2**. Second tier of Student Interaction Discourse Moves (SIDM) Analytical Framework codes – Primary Intent. (Table 2 in (Nennig et al., 2023))*

Primary Intent: describes for what purpose the student is speaking

Discourse Move	Definition
Acknowledging (AL)	Recognizing a stated utterance that does not meaningfully contribute to the conversation
Commenting (CM)	Personal remarks, the judgment of activity/class, or utterances of how students understand the material or future plans to work on material
Concluding (C)	Statements that serve as a consensus and ends the question answering process
Contributing to Discussion (RC)	Responses that contribute to the completion of the activity
External Interaction (EI)	Interactions that take place with someone who is not a member of the group or instructor
Initiating (I)	Students begin to work on the activity prompt
Managing (MG)	Management of time, works tasks, and student roles or utterances related to getting started to begin the activity
Questioning (Q)	Utterances that require member(s) to respond during the activity (does not include questions regarding management of time or work tasks)

***Table S3**. Third tier of Student Interaction Discourse Moves (SIDM) Analytical Framework codes – Nature of Utterance. (Table 3 in (Nennig et al., 2023))*

Nature of Utterance: describes the manner students engage in a specific discourse move

Discourse Move	Definition
Activity Prompt (AP)	Reading the activity prompt out loud
Agreeing (A)	Voicing agreement to a previous utterance
Assessing (AS)	Determining if the strategy addresses all aspects of the problem/task and is functional or if an answer makes sense
Building (B)	Completing an incomplete utterance or expanding on an utterance with more detail or adding additional claims. (This is coded along with another code to describe the nature of the building utterance.)
Clarification Seeking (CL)	Requesting clarification of what another student said or what is being stated or confirming their interpretation is correct
Explanation Seeking (E)	Requesting another student to share ideas, seeking an initial answer to a question or how to think about a problem, or requesting backing to a claim
Information Processing (IP)	Evaluating, interpreting, or transforming given information (students trying to make sense of given information)
Information Seeking (IS)	Requesting for more information needed to solve the problem such as conversion factors, definitions, or rules
Motivating (M)	Providing encouragement to group members
Organizing (O)	Getting ready to work on the task, making sure members are working on the correct task, keeping up with discussion, or assignment of student roles/tasks
Past Experiences (PE)	Describing experience(s) with science
Personal Remarks (PR)	Describing current state of being, or how they feel about the activity, prompt, something they need to complete or other comments not related to completing the task
Presenting a Claim (PC)	Suggesting an answer (may be tentative in nature)
Procedural (P)	Describing how to solve the problem. This can include the calculational process
Providing Information (PI)	Conveying an idea that is needed to solve the problem (ex. conversion factors, definitions, rules, formulas, data) or move the conversation forward
Reasoning (RS)	Thinking through the problem/scenario or justifying or supporting an idea with scientific reasoning
Rebutting (RB)	Rejecting an assertion supported with reasoning
Rejecting (RJ)	Explicitly voicing disagreement with an utterance
Repeating (RP)	Revoicing an utterance that has been previously stated
Reporting (RT)	Revoicing an idea or feedback to move the conversation forward
Summarizing (SM)	Summarizing ideas or steps to solve a problem that arose from the conversation

Non-Verbal Interaction (NVI)	Contributing to the completion of the activity by engaging in conversation without words. (This is coded along with another code to describe the nature of the non-verbal utterance.)
Not Audible or Applicable (N/A)	Utterances that are inaudible due to static or are not appropriately described by any of the proposed codes

Key of colors, symbols, and markers used to construct the discourse maps

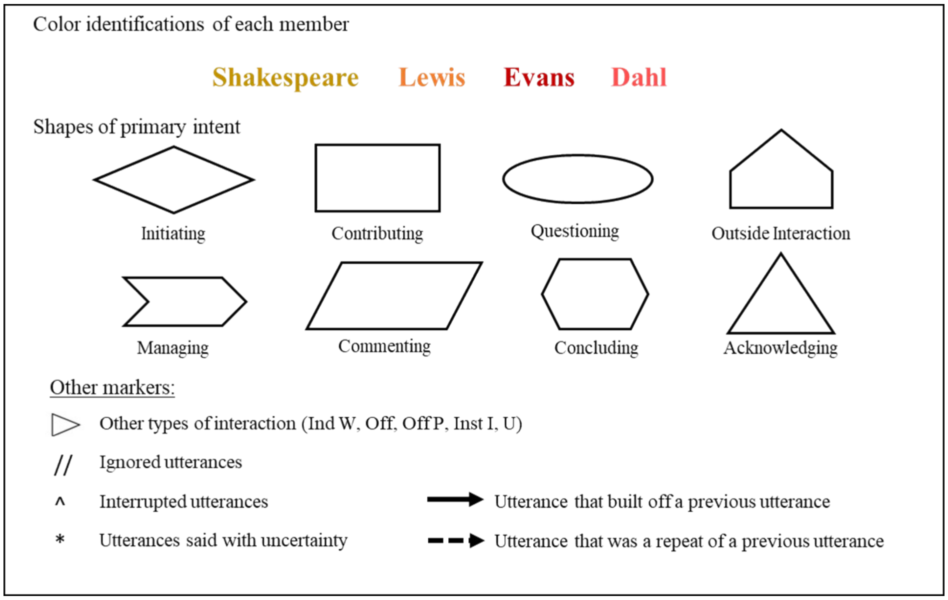


***Fig. S3**. Key of colors, symbols, and markers used to construct the SIDM discourse maps (Modified from Figure 2 in (Nennig et al., 2023) with permission from authors)*

Transcript with applied SIDM codes

SIDM was applied to determine the social and cognitive engagement of groups while working on a given task. For each utterance transcribed in the student group conversation the authors applied the three-tier SIDM framework layer by layer, starting with Type of Interaction, Primary Intent, and ending with Nature of Utterance. Below in Table S4. the coding that was applied to the example conversation discussed in the manuscript (Figures 1-5) has been provided.

***Table S4**. Transcribed conversation between Shakespeare, Lewis, Evans, and Dahl with applied SIDM coding.*

Utterance Number	Student	Utterance	Type of Interaction	Primary Intent	Nature of Utterance
1	**Shakespeare:**	Basically, one electron from the 1s goes away and one of the electrons from the 2p replaces it by going down to the 1s.	On-Task	Initiating	Activity Prompt, Interrupted
2	**Lewis interrupts Shakespeare:**	Okay so it goes from…	On-Task	Contributing to Discussion	Not Applicable
3	**Shakespeare:**	Because you need to fill it back up	On-Task	Contributing to Discussion	Information Processing
4	**Lewis:**	$2p^6$ to $2p^5$ to replace the…	On-Task	Contributing to Discussion	Presenting a Claim, Building on Utterance 1
5	**Shakespeare:**	To replace the 1s which has lost energy.	On-Task	Contributing to Discussion	Reasoning, Building on Utterance 4, Interrupted
6	**Lewis interrupts Shakespeare:**	…the one that lost an electron.	On-Task	Contributing to Discussion	Presenting a Claim, Building on Utterance 4
7	**Shakespeare:**	Yup	On-Task	Contributing	Agreeing

		And then that process emits a photon basically.	On-Task	to Discussion Contributing to Discussion	Presenting a Claim
8	**Evans:**	*huff*	On-Task	Commenting	Personal Remark
9	**Lewis:**	[*Lewis starts interaction with TA.Hermione about their answer to the previous task.*]	Instructor Interaction	-	-
10	**Shakespeare:**	Ah for that ummm draw these in like you did last time.	On-Task	Managing	Organizing
11	**Evans:**	All of them?	On-Task	Questioning	Clarification Seeking
12	**Shakespeare:**	Just for the first diagram.	On-Task	Contributing to Discussion	Organizing
		So the 1s would have two electrons, 2s would have two electrons.	On-Task	Contributing to Discussion	Presenting a Claim
13	**Evans:**	And then 6 here? [*Pointing at 2p orbital*]	On-Task	Questioning	Clarification Seeking
14	**Shakespeare:**	Yup.	On-Task	Contributing to Discussion	Agreeing
		And then for that one, 2s is going to be the same	On-Task	Contributing to Discussion	Presenting a Claim
15	**Dahl:**	I was listening to [*TA. Hermione*]. What problem are we working on?	On-Task	Managing	Information Seeking, Ignored Utterance
16	**Shakespeare directed at Evans:**	And then 2p is going to have five electrons instead of six, so the last one would just have one. And then 1s is going to have two.	On-Task	Contributing to Discussion	Presenting a Claim
17	**Evans:**	But then wouldn't it have to be…	On-Task	Questioning	Clarification Seeking
18	**Dahl:**	So what question?	On-Task	Questioning	Repeating Utterance 15, Ignored Utterance
19	**Evans:**	So instead of … [*pause*]	On-Task	Contributing to Discussion	Not Applicable
20	**Shakespeare:**	It says, knock out an electron from 1s, and then put one of the electrons from 2p where that 1s electron was, so everything looks the same except this is five instead of six.	On-Task	Contributing to Discussion	Repeating Utterance 12
21	**Evans:**	What does that…	On-Task	Questioning	Explanation Seeking, Interrupted
22	**Shakespeare interrupts Evans:**	And then you released a photon.	On-Task	Managing	Procedural
23	**Evans to Shakespeare:**	Like that? [*Pointing to what they drew and wrote.*]	On-Task	Questioning	Clarification Seeking
24	**Dahl:**	Yeah	On-Task	Contributing to Discussion	Agreeing
25	**Shakespeare:**	Photon not proton.	On-Task	Managing	Rejecting
26	**Evans:**	*Giggles* [*Erases proton and changes it to photon.*]	On-Task	Acknowledging	Non-Verbal Interaction
27	**Lewis to TA.Hermione**	Thank you!	Instructor Interaction	-	-

Detailed application of Student Expressed Chemical Thinking (SECT) maps to transcript conversation from Figure 1-5 in main manuscript.

SECT Code Book.

SECT maps were generated from transcripts of student group conversations by first identifying the main chemical concepts and ideas expressed by students in a group, and depicting how they were connected during conversation. This analysis allowed us to segment each transcript into sections in which students engaged in a particular cognitive process or a set of cognitive processes directed by a particular goal. The following code book includes the main three code categories along with the most common cognitive processes applied in the observed tasks:

Table S5. *Code definitions for SECT maps.*

Code	Definition	Key Features
Chemical Content	Key chemical ideas uttered by students during their conversation while working on a given task	• Must include chemical information • Can be stated as a fact or question • Can be restated information previously provided from other students, instructors, or materials

Consensus Outcome	A summary statement or behaviour that represents the outcome of chemical ideas discussed for a particular portion of student group dialog	• Statement by students that clearly wraps up a portion of dialog
		    ○ Can be final answer or intermediate step
		• Behaviour that would pause or end a portion of dialog, such as writing or drawing the piece of an answer
		    ○ Can be final answer or intermediate step
		• Occurs most often near the end of a Cognitive Process
		    ○ Can occur at any time in a conversation
		    ○ On rare occasions more than once
		    ○ May not occur at all

Cognitive Process	Describes the nature of chemical thinking occurring for a particular portion of student group dialog	See Table S6.

Table S6. *Code definitions for types of Cognitive Process for SECT maps.*

Code	Definition	Key Features
Calculating	When students determine a value or engage in quantitative reasoning to come up with a number	Student must determine a numerical value for their response, whether that be entered in free response or selecting a multiple-choice value.
Describing	When students generate dialog regarding what is happening in a system or phenomenon	Students making a statement of meaning about the system or phenomenon under analysis, such as providing a definition.
Explaining	When students use scientific principles/concepts in their dialog as to why a property, behaviour, or phenomenon is true or how it works	Students justify behaviours using associating properties and/or build causal links between events.
Interpreting	When students make meaning of information that is explicitly presented while conversing	Students extracting information from a graph or diagrams or written text to make sense of the task.
Inferring	When students connect information that involves building relationships among properties or determining patterns of behaviour from analysed information while conversing	Students discussing trends they've identified in the provided information to have something done to them to determining properties or behaviours from explicit or implicit cues in a task.
Modelling	When students develop or start to develop a sense-making tool that helps explain or predict the natural world while conversing	Students communicating potentially how theoretical ideas connect to the model under study.
Predicting	When students make an educated guess about a behaviour that incorporates making inferences about the products	Students determining relative values of properties or quantitative values from analysis of numerical data. Students making qualitative predictions about properties or behaviours.
Representing	When students converse changing one	Students constructing representation to or from text,

	representation type into another. It does not matter what form the representation starts in, just that the students are changing one form into another form.	equations, 2D models, 3D models or other forms. Drawing or verbally conveying representations of chemical substances, processes or systems are a few examples.
Summarizing	When students review or summarize their ideas, conclusions, or answers.	Students recapitulating ideas, agreed answer, and/or reasoning already mentioned in previous utterances.

Transcript with applied SECT codes

For each of these segments we also identified the outcome of students' cognitive process by analyzing the specific intellectual products of their work. As an example, consider the following analysis of the transcript in Table S7. associated with the group activity corresponding to Figs. 1 through 5 in the main manuscript.

Table S7. *Transcribed conversation between Shakespeare, Lewis, Evans, and Dahl with applied SECT coding.*

Utterance Number	Student	Utterance	SECT Major Segments
1	**Shakespeare:**	Basically, one electron from the 1s goes away and one of the electrons from the 2p replaces it by going down to the 1s.	A student explains how light is emitted by transference of an electron from a higher to a lower energy orbital. **Cognitive Process:** Explaining **Consensus Outcome:** Generation of an explanation for how light is emitted
2	**Lewis interrupts Shakespeare:**	Okay so it goes from…	
3	**Shakespeare:**	Because you need to fill it back up	
4	**Lewis:**	$2p^6$ to $2p^5$ to replace the…	
5	**Shakespeare:**	To replace the 1s which has lost energy.	
6	**Lewis interrupts Shakespeare:**	…the one that lost an electron.	
7	**Shakespeare:**	Yup And then that process emits a photon basically.	
8	**Evans:**	*huff*	Students build a representation of the location of electrons in the electron-energy diagram before X-ray absorption. **Cognitive Process:** Representing **Consensus Outcome:** Completion of first electron-energy diagram
9	**Lewis:**	[*Lewis starts interaction with TA.Hermione about their answer to the previous task.*]	
10	**Shakespeare:**	Ah for that ummm draw these in like you did last time.	
11	**Evans:**	All of them?	
12	**Shakespeare:**	Just for the first diagram. So the 1s would have two electrons, 2s would have two electrons.	
13	**Evans:**	And then 6 here? [*Pointing at 2p orbital*]	
14	**Shakespeare:**	Yup. And then for that one, 2s is going to be the same	
15	**Dahl:**	I was listening to [*TA. Hermione*]. What problem are we working on?	Students build a representation of the location of the electrons in the electron-energy diagram after X-ray absorption. **Cognitive Process:** Representing **Consensus Outcome:** Completion of second electron-energy diagram
16	**Shakespeare directed at Evans:**	And then 2p is going to have five electrons instead of six, so the last one would just have one. And then 1s is going to have two.	
17	**Evans:**	But then wouldn't it have to be…	
18	**Dahl:**	So what question?	
19	**Evans:**	So instead of … [*pause*]	
20	**Shakespeare:**	It says, knock out an electron from 1s, and then put one of the electrons from 2p where that 1s electron was, so everything looks the same except this is five instead of six.	A student recapitulates what happens during the analysed process **Cognitive Process:** Summarizing **Consensus Outcome:** Clarification and restatement of the characteristics of the final
21	**Evans:**	What does that…	
22	**Shakespeare interrupts Evans:**	And then you released a photon.	
23	**Evans to Shakespeare:**	Like that? [*Pointing to what they drew and wrote.*]	

24	**Dahl:**	Yeah	products (two electron-energy diagrams); completion of drawing
25	**Shakespeare:**	Photon not proton.	
26	**Evans:**	*Giggles* [*Erases proton and changes it to photon.*]	
27	**Lewis to TA.Hermione**	Thank you!	

Mapping of SECT coding from the transcribed conversation

In this case, the transcript was segmented into four major sections involving different cognitive processes. The segments were then visually represented in the corresponding SECT map shown below. In this map, the blue boxes summarize the chemical content uttered by students while working on the task. These utterances are separated into groups or segments, encapsulated within the black dotted lines, based on the type of cognitive process in which students were. Yellow boxes below each group are used to indicate consensus outcomes of each activity.

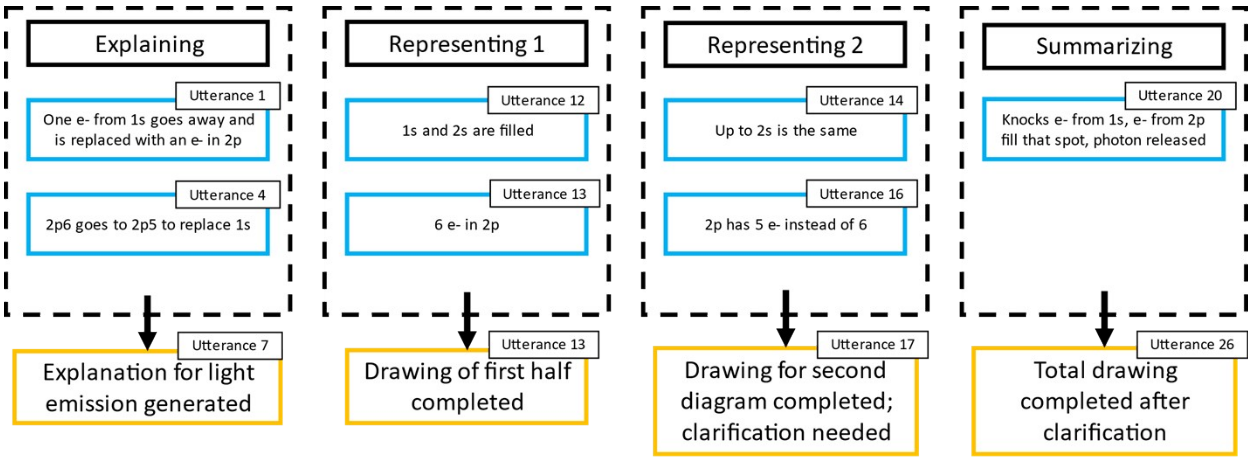


Figure S4. *SECT map presented in manuscript as Fig. 3, relates to conversation from Figs. 1-5 in manuscript.*

Generating CoL circle maps from SIDM-SECT maps

In this section we exemplify how the authors analyzed each of the SIDM-SECT combined maps to build the Community of Learners (CoL) circle maps. As mentioned in the manuscript, the five dimensions of CoL were visually represented using colored circles. Each dimension was assigned a circle and a color, except for the dimension of Community of Practice (CoP), which was split into two subdimensions with their own respective circles. All dimension circles were then subdivided into equal sectors to represent each group member present during the conversation for which the SIDM-SECT map was constructed. These circle sectors were filled in if the corresponding group member engaged and contributed during the conversation as determined by the lens of each dimension. If the student participating in the conversation did not meet the given criteria of the related dimension, that circle sector was only outlined. Sectors corresponding to students not explicitly engaged in the conversations were left completely blank for all dimensions.

In Fig. S5 below, which corresponds to Fig. 4 and Fig. 5 in the manuscript, we make explicit using rectangles, the different sections on the SIDM-SECT where we found evidence of engagement in the different dimension of analysis in the CoL framework. The color of the rectangles is indicative of the dimension in the CoL framework for which the selected section of the conversation provided evidence. Through this analysis, we identified which students contributed to the conversation, when, and how as described in the sections below. The dimension CoD (blue color) is not explicitly shown on the image as engagement in this dimension was inferred from the analyses of all utterances.

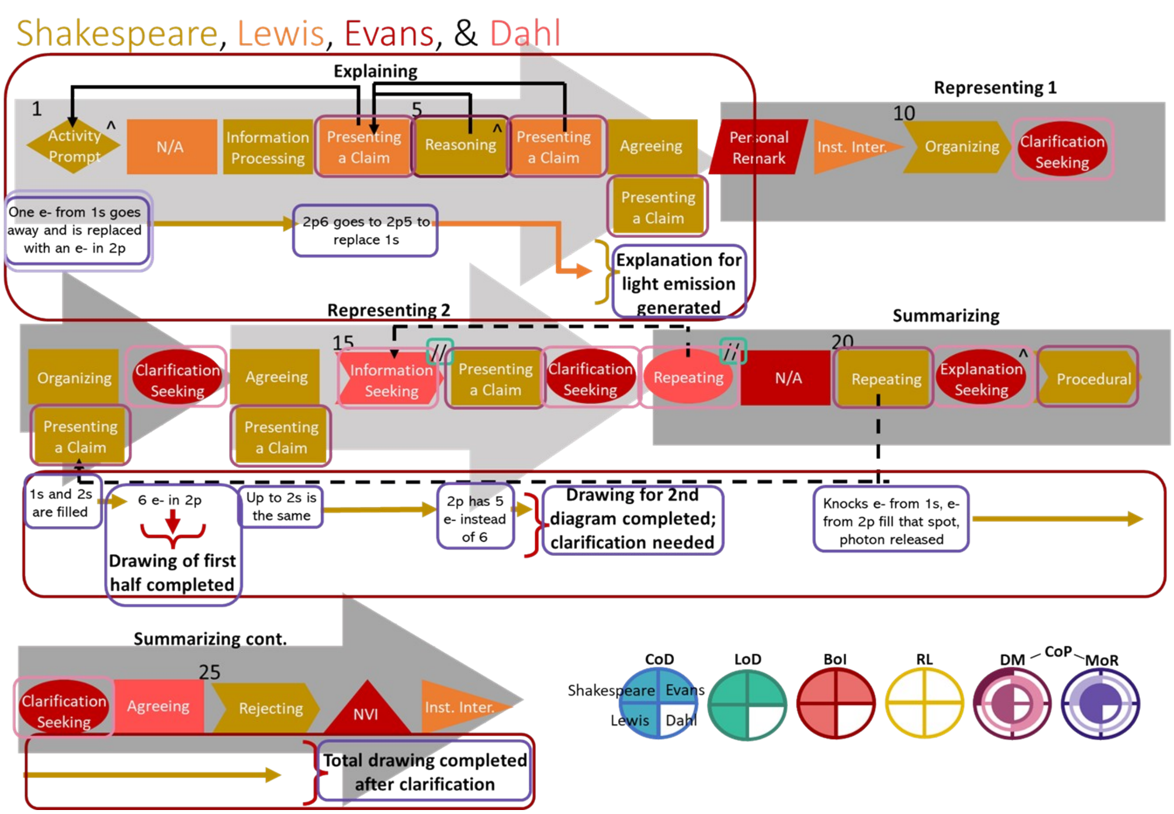


Fig. S5 Annotated SIDM-SECT map.

A. Community of Discourse (CoD)

For this dimension the outline of each group member's sector of the circle was determined based on their participation. If a group member was conversing on-task with the rest of the group beyond the discursive moves of agreeing and acknowledging, their sector of the circle was outlined. An example of this can be seen in Fig. S5, where all four group members contributed to the conversation and have earned this outline. For group members not meeting these criteria, their circle sector was not outlined, and remained missing across the other dimensions. An example of this can be seen in the Appendix Case Study 3 Group D (Table. A3), where Brittany's portion of the circle is missing across all the dimensions, even though they are physically present throughout the conversation. After outlining the CoD circle, the filled in color of the circle sector represents which students are moving the conversation forward through the use chemical ideas.

B. Legitimization of Differences (LoD)

This dimension highlights the extent to which the contributions of group members are acknowledged, discussed, and considered in the construction of understandings. This dimension is represented using a green circle with filled sectors for those group members whose contributions were acknowledged and used to complete the task. This was determined in the SIDM-SECT combined map by looking for instances of ignored, interrupted, rejected, or rebutted utterances. First, if a group member was ignored at any point in the conversation, immediately that group member was characterized as being left out by the rest of the group. This was the case for Dahl at utterances 15 and 18 in Fig. S5 where both of Dahl's utterances are marked with the double backslash symbol, which represents when an utterance has been ignored. Second, for occurrences of interrupted utterances, the number of interrupted utterances and who prompted those interruptions were tracked throughout a conversation. If one group member was interrupted multiple times by the same or multiple group member(s), that interrupted group member was characterized as being left out. However, for conversations where interruptions were a common occurrence amongst all group members, these interruptions were deemed as characteristic of how the group communicated and not intended to leave someone out. The third type of utterances monitored from the SECT-SIDM combined maps for the LoD dimension were rejecting and rebutting. Though these types of utterances are typically seen as productive forms of student engagement with chemical ideas, these moves can also shut down group members from participating if their ideas are continuously rejected throughout a conversation. For this reason, how often each group member was rejected or rebutted in a conversation was tracked. If there was evidence that a particular group member was hindered from participating in this way, their sector of the LoD circle was left unfilled.

C. Building on Ideas (BoI)

This dimension denotes which group members were participating in a decentered conversation with multiple members building chemical ideas off one another. Annotations in the SIDM-SECT combined maps that helped determine this dimension included black building arrows tying utterances from one group member to another and/or periods of conversation where group members shared chemical content that build on previously stated chemical content as represented by the interchanging-colored arrows. The occurrence of one or both of these annotations in the SIDM-SECT maps by a group member resulted in a filled sector of the BoI red circle. An example of this can be seen in Fig. S5 during the Explaining portion of the conversation between Lewis and Shakespeare. Both group members are constructing an answer together using chemical concepts as annotated with the black building arrows as well as the alternating gold and orange arrows. Another example of this phenomena occurs later in the same conversation but between Evans and Shakespeare. During Representing 2 and Summarizing, Evans and Shakespeare both build chemical content off one another as evident with the alternating gold and maroon arrows, with Evans also constructing consensus products from their conversation at utterances 13, 17, and 26 as indicted with the maroon braces.

D. Reflective Learning (RL)

This dimension highlights which group members engaged in self-motivated, reflective, and purposeful learning through the discursive moves of past experience, reporting, motivating, and/or assessing. Group members characterized with these types of utterances in the SIDM-SECT combined maps are represented with a filled yellow sector of a circle. The conversation diagramed in Fig. S5 does not depict group members participating in any of these discursive moves, therefore the dimension circle remains just an outline for each group member. An example of RL is observed in the Appendix Case 1 Group A (Table. A1), where Charlie is seen engaging in the discursive move of assessing during utterance 34, resulting in a filled yellow sector.

E. Community of Practice (CoP)

This dimension characterizes the extent to which group members engaged in authentic intellectual work in the discipline through the communication of chemical ideas and different types of reasoning.

The first subdimension of CoP is Community of Practice - Discourse Moves (CoP-DM), characterizes group members' engagement in the conversation through various discourse moves. As with prior representations for other dimensions, a filled sector was used to indicate a member's engagement with the practice while the sectors for non-contributing individuals were just outlined. For the CoP-DM pillar (in pink), the center of the bullseye colored in represents when students are sharing information, using the following discursive moves: presenting claims, providing information, and/or providing procedural information. The middle ring of the bullseye represents the group members who have asked questions during the conversation, while the outside ring represents the students who have provided discursive moves of reasoning or rebutting (which are rejections with reasoning). An example of this can be seen in Fig. S5 where throughout the conversation Shakespeare presented claims (utterance 7, 12, 14, and 16) and procedural information (utterance 22) as well as provided reasoning (utterance 5), these discursive moves are represented by the center of his portion of the bullseye being filled in along with the outside edge. Throughout the conversation Shakespeare never asks a question, resulting in an unfilled middle sector of the CoP-DM bullseye.

The second subdimension of the CoP is Community of Practice – Modes of Reasoning (CoP-MoR), characterizes students' use of chemical reasoning. The inner ring of CoP-MoR pillar (in purple) represents descriptive reasoning based on stating and contributing pieces of chemical knowledge to the conversation, the middle ring associated with relational reasoning strongly reliant on rules or associative heuristics to connect concepts or ideas, and the outer ring representing engagement in model-based reasoning in which students explicitly expressed causal links while connecting ideas. An example of how this was applied can be seen in Fig. S5, during the Explaining segment, where Shakespeare uses relational reasoning as he is expressing a sequence of ideas that are going from one place to another.

Results from Chi-Square tests and analysis of residuals for data in Table 3 in the main manuscript

Table S8. *Results from Chi-Square tests and analysis of residuals for data in Table 3 in the main manuscript.*

Number of conversations in each category in parenthesis		CoD	LoD	BoI	RL	CoP-DM			CoP-MoR		
						Sharing	*Asking*	*Justifying*	*Descriptive*	*Relational*	*Model-based*
Group Size	*2 (8)*	100+	100	68.8-	6.3-	75.0	87.5	56.3	100+	50.0+	12.5+
	3 (18)	88.9	90.7	74.1	38.9+	75.9	77.8	50.0	83.3	40.7	3.7-
	4 (37)	79.7	85.8	70.9	25.7	67.6	75.7	45.9	74.3	39.2	4.1
	5 (3)	66.7-	86.7	73.3	33.3+	60.0	80.0	40.0	60.0-	26.7-	0-
Cognitive Level	*Retrieval (6)*	90.3+	84.7	73.6	13.9-	56.9-	80.6	58.3+	74.7+	37.5	0-
	Comprehension (30)	83.3	91.4	72.3	30.0+	75.2+	77.4	46.2	77.9	33.8-	0-
	Analysis (30)	83.5	87.6	71.5	28.3	68.7	78.5	48.2	79.5	46.6+	10.2+
Task Type	*Calculation (10)*	75.3	89.7+	65.2	42.5+	72.0+	83.8+	37.7-	67.0-	18.7-	0-
	Comparison (12)	79.6	87.9	67.5	19.4-	71.0	71.0	48.8	71.7-	53.6+	4.2
	Representation (8)	86.5	89.6	76.0	42.7+	76.0	72.9-	52.2	86.5	35.4-	0-
	Inf./Int./Expl. (34)	86.8	88.2	72.3	19.2-	66.7-	78.4	51.0	82.6	45.6+	7.8+
Overall		84.1	88.9	71.6	27.3	70.4	77.9	48.0	79.2	40.4	4.8

Chi-Square Analysis

We report values of standardized residuals for items in each category of analysis. If the residual is less than -2, the cell's observed frequency is less than the expected frequency. Greater than 2 and the observed frequency is greater than the expected frequency).

Table S9. *Chi-Square Analysis for Group Size.* $\chi^2 = 630.03$*, df = 30, p-value* $< 2.2 \times 10^{-16}$

Number of conversations in each category in parenthesis		CoD	LoD	BoI	RL	CoP-DM			CoP-MoR		
						Sharing	*Asking*	*Justifying*	*Descriptive*	*Relational*	*Model-based*
Group Size	*2 (8)*	2.439	0.862	-3.008	-12.187	-0.585	0.778	1.505	4.122	2.550	8.971
	3 (18)	0.278	-1.145	-0.559	8.135	1.004	-1.865	-0.250	0.070	-1.064	-2.493
	4 (37)	-0.824	0.147	1.455	-0.686	-0.156	0.497	-0.259	-1.363	0.340	-1.611
	5 (3)	-2.105	0.935	1.587	2.851	-1.026	1.711	-1.090	-2.616	-2.971	-3.64

Number of conversations in each category in parenthesis		CoD	LoD	BoI	RL	CoP-DM			CoP-MoR		
						Sharing	*Asking*	*Justifying*	*Descriptive*	*Relational*	*Model-based*
Cognitive Level	*Retrieval (6)*	2.241	-0.536	1.290	-6.062	-3.447	1.284	4.114	2.064	-0.721	-5.301
	Comprehension (30)	-0.031	1.905	0.557	3.112	3.503	0.136	-1.108	-0.391	-5.408	-11.954
	Analysis (30)	-0.952	-1.649	-0.919	-0.419	-1.953	-0.698	-0.708	-0.518	5.666	14.151

Table S10. *Chi-Square Analysis for Cognitive Level.* $\chi^2 = 557.23$*, df = 20, p-value* $< 2.2 \times 10^{-16}$

Number of conversations in each category in parenthesis		CoD	LoD	BoI	RL	CoP-DM			CoP-MoR		
						Sharing	*Asking*	*Justifying*	*Descriptive*	*Relational*	*Model-based*
Task Type	*Calculation (10)*	-1.333	2.052	-0.658	11.61	2.456	4.001	-4.018	-2.685	-10.422	-6.844
	Comparison (12)	-0.780	0.533	-0.658	-3.97	1.328	-1.741	0.447	-2.005	7.0045	-1.055
	Representation (8)	-0.320	-0.926	0.623	8.570	1.068	-2.508	1.543	1.303	-3.515	-6.442
	Inf./Int./Expl. (34)	1.311	-0.929	0.422	-7.99	-2.588	0.156	1.083	1.934	3.085	7.378
Overall		84.1	88.9	71.6	27.3	70.4	77.9	48.0	79.2	40.4	4.8

Table S11*. Chi-Square Analysis for Task Type.* $\chi^2 = 753.76$, *df* = 30, *p-value* $< 2.2 \times 10^{-16}$

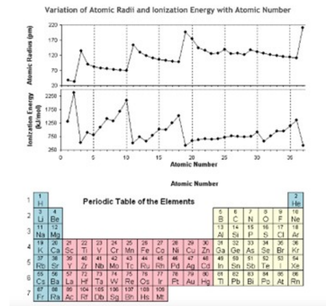
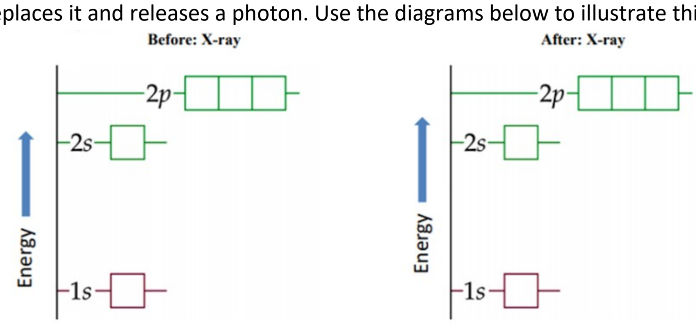
Marzano Codebook

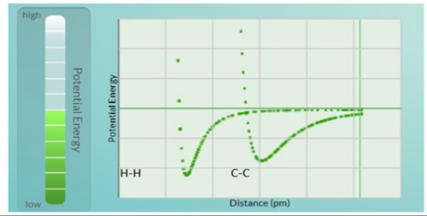
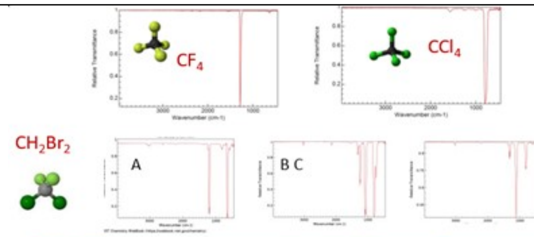
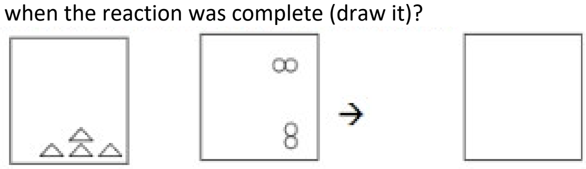
Table S12. *Definitions of Cognitive Level of a Task from Marzano's Taxonomy (Modified from Table 6 in (Reid* et al.*, 2022))*

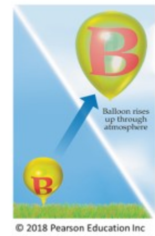
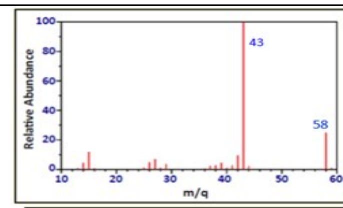
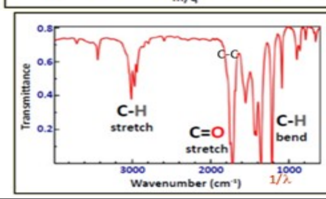
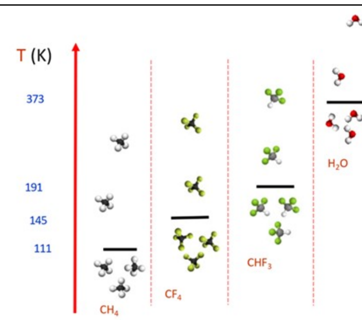
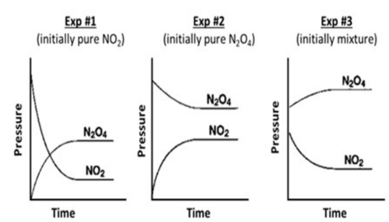
Cognitive Level of a Task: describes the mental process of applying knowledge and/or understanding to complete a task.

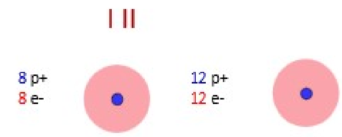
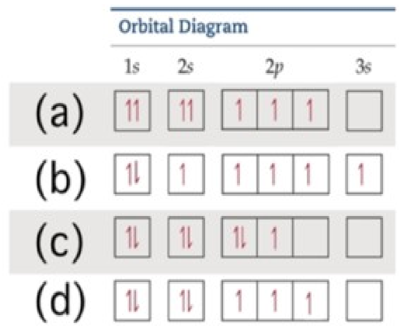
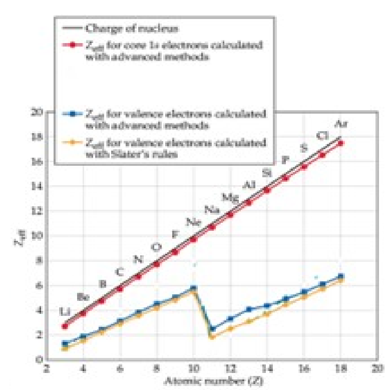
Level	Definition	Example
Retrieval	Involves the simple recognition, recall, or execution of knowledge, including rote calculations. Tasks of this level ask a learner to reiterate or identify information in almost the exact way it was introduced	How is atomic radius defined?
Comprehension	Involves the integration and symbolic representation of knowledge, generally with a focus on key features and organization of information	Explain how you determine if a bond is polar and the direction of a bond dipole.
Analysis	Involves examining knowledge in detail and generating new conclusions	Consider substances made up of the following atoms and molecules: He, CH_4, Ne, C_2H_6. Arrange the substances in order of increasing boiling point and clearly justify your rankings
Knowledge Utilization	Requires that students apply or use knowledge in specific situations and almost always includes a component of justification. These tasks will include decision making between two or more alternatives, problem solving that includes accomplishing goals for which an obstacle exists, experimenting, or investigating	Based upon everything you have learned; do you think that solar geoengineering should be an option for combating climate change? Justify your answer

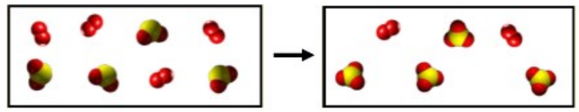
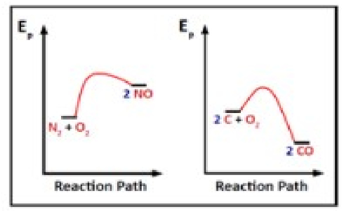
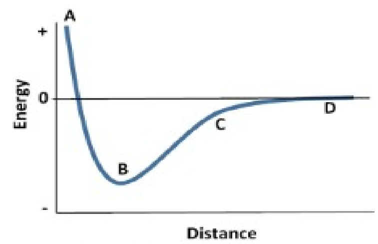
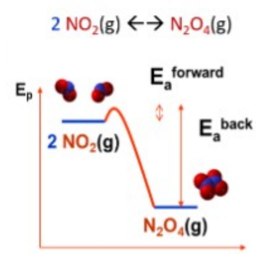
All tasks assessed throughout this study.

Task Characterization	Task
Question Format: Free Response **Cognitive Level of Task:** Comprehension **Type of Task:** Calculation/Interpretation	A single oxygen – 16 atom has a mass of 16.00 amu. Convert this mass to grams, and then calculate the mass in grams of a mole of oxygen – 16 atoms. Based on your results for exercises one and two, identify the relationship between the numerical values of the mass of the atom in amu and the molar mass in g/mol.
Question Format: Free Response **Cognitive Level of Task:** Analysis **Type of Task:** Explanation/Comparison	As the atomic number increases across a row in the periodic table, does the electron-nucleus attraction for an electron increase or decrease, and what effect would this have on radii (r) and ionization energies (IE)? 
Question Format: Multiple Choice/Rank **Cognitive Level of Task:** Comprehension **Type of Task:** Comparison	Consider F^-, Ne, and Na^+. How should the radii of F^-, Ne, and Na^+ compare? ● $F^- < Ne < Na^+$ ● $F^- < Na^+ < Ne$ ● $Ne < F^- < Na^+$ ● $Ne < Na^+ < F^-$ ● $Na^+ < F^- < Ne$ ● $Na^+ < Ne < F^-$
Question Format: Free Response **Cognitive Level of Task:** Comprehension **Type of Task:** Calculation	If a gas in a sealed jar (V constant) is heated to the Kelvin temperature doubles, by what factor does the pressure change? Enter a numerical answer. For example, if it triples enter a 3. If it is reduced by a third, enter 0.33. Factor = ______
Question Format: Draw **Cognitive Level of Task:** Comprehension **Type of Task:** Representation Transformation	For X-ray fluorescence, the material is exposed to high-energy X-rays that knock out a core electron and then an electron from a higher energy orbital moves into that lower energy state. When that happens, a photon is released. Let's say that when the X-rays hit the ferro-gallus ink, it knocks out an electron from the 1s orbital and an electron from the 2p orbital replaces it and releases a photon. Use the diagrams below to illustrate this process. 
Question Format: Free Response **Cognitive Level of Task:** Comprehension **Type of Task:** Interpretation/Calculation	**Stuff to know: q=mcΔT** Heat of fusion of water = 334 J/g, Heat of vaporization of water = 2257 J/g, Specific heat of ice = 2.06 J/g·°C, Specific heat of liquid water = 4.18 J/g·°C, Specific heat of steam = 2.02 J/g·°C, Specific heat of ethanol = 2.44 J/g·°C What is the heat in Joules required to convert 25.00 grams of ice at -10.0°C to 150.0°C steam?
Question Format: Matching **Cognitive Level of Task:** Analysis **Type of Task:** Inference	**Matching** Identify each energy exchange as heat or work and determine whether the sigh of heat or work (relative to the system) is positive or negative. A. An ice cube melts and cools the surrounding beverage (the ice cube is the system) B. A metal cylinder is rolled up a ramp (the cylinder is the system) C. Steam condenses on skin, causing a burn (steam is the ystem) 1. Heat, Positive 2. Work, Positive 3. Heat, Negative

Question Format: Free Response **Cognitive Level of Task:** Analysis **Type of Task:** Comparison	**Let's Think** Which chemical bond is longer? Which chemical bond is stronger? 
Question Format: Free Response **Cognitive Level of Task:** Analysis **Type of Task:** Explanation/Inference	As we take a breath, the diaphragm muscles move down and the volume of our lungs increase. Assuming that there is a fixed quantity of gas in your lungs and the temperature remains constant, what happens to the pressure? Why does this allow us to inhale?
Question Format: Multiple Choice **Cognitive Level of Task:** Comprehension **Type of Task:** Interpretation	**Let's Think** Which IR spectrum corresponds to this substance? 
Question Format: Multiple Selection **Cognitive Level of Task:** **Type of Task:** Interpretation/Inference	**Many Choice** In the laboratory, a student dissolves a quantity of solid ammonium chloride, NH_4Cl, in 50.0 mL of water in a coffee-cup calorimeter. The initial temperature of the water was 21.5 °C, and the final temperature of the aqueous solution of ammonium chloride was 19.3 °C. Which statements about this experiment are true? A. The dissolution of ammonium chloride is an endothermic process. B. The dissolution of ammonium chloride is an exothermic process. C. ΔT for the system is greater than 0. D. ΔT for the surroundings is greater than 0. E. The system gained heat during the process. F. The surroundings gained heat during the process.
Question Format: Free Response **Cognitive Level of Task**: Comprehension **Type of Task:** Calculation	**Model 2: Particulate and Molar View: A reaction of Sodium.** Consider the reaction of sodium metal reacts in aire to form sodium oxide solid (demostration). *Key Questions* If the reaction is takes place using the starting materials depected below where sodium is represented by ▲ and oxygen molecules are represented by ꝏ what would be in the reaction vessel when the reaction was complete (draw it)?  Let's run the reaction in question 10 with more particles. How many dozen sodium oxide units would you make if you started with 8 dozen atoms of sodium and 4 dozen molecules of oxygen?
Question Format: Free Response **Cognitive Level of Task:** Analysis **Type of Task:** Definition/Comparison	What are some of the characteristics (ie ductile, brittleness, hardness) of the material that you defined in question 2 and how does that relate to what you know about bones? [*Question 2: The major mineral phase is a calcium phosphate mineral called hydroxyapatite ($Ca_5(PO_4)_3(OH)$). Is this a metallic, ionic or molecular structure? What kind of interactions informed your answer?*]

Question Format: Multiple Selection **Cognitive Level of Task:** Analysis **Type of Task:** Inference	**Learning Catalytics – A balloon rising through the atmosphere increases in volume. Which of the following statements is true?** A: Atmospheric pressure rises causing the balloon to expand. B: Atmospheric pressure falls causing the balloon to expand. C: Gases expand when heated and so the atmosphere gets warmer the higher up you get. D: The balloon must be completely sealed because otherwise it would shrink. 
Question Format: Free Response **Cognitive Level of Task:** Comprehension **Type of Task:** Representation Transformation	**Exercises.** The basic ham and cheese sandwich will be defined here as 2 slices of bread (B), a slice of ham (H), 2 slices of cheese (C) and a slice of tomato (T). (You may not agree with me but humour me in the name of an example). Write a "chemical reaction" for making a ham sandwich using the symbols given in the recipe.
Question Format: Free Response **Cognitive Level of Task:** Analysis **Type of Task:** Interpretation	**Let's Think** IR/MS breath analysis can be used to explore fat metabolism for people on a diet. The metabolism of fat produces a volatile compound with the formula C_3H_6O. **Propose a molecular structure for this compound consistent with the data.**  
Question Format: Free Response **Cognitive Level of Task:** Comprehension **Type of Task:** Representation Transformation/Interpretation	When the water flows through the pipe, you will also get a reaction between dissolved lead (II) cations located near the surface of the lead pipe and dissolved calcium carbonate to form solid lead (II) carbonate. What type of reaction is this? Write the complete ionic equation for this reaction and the net ionic equation. What is the spectator ion in this case?
Question Format: Free Response **Cognitive Level of Task:** Analysis **Type of Task:** Inference	**Let's Think** Make a list of differentiating characteristics that may be responsible for the different boiling points of these four substances. 
Question Format: Multiple Selection **Cognitive Level of Task:** Comprehension **Type of Task:** Interpretation	**LC.** Response system gives A, B, C, D options and says choose all that apply. Consider 3 experiments to study: N_2O_4 (g) ⇌ 2 NO_2 (g) each with a different startng point. *For which the following experiments is the system at equilibrium?* 

Question Format: Free Response **Cognitive Level of Task:** Analysis **Type of Task:** Comparison	**Let's Think** Consider this pair of particles: Which is more polarizable? Why? 
Question Format: Multiple Selection **Cognitive Level of Task:** Comprehension **Type of Task:** Inference	Given the following reaction, how could you increase the concentration of products? Select all that apply. N_2 (g) + $3H_2$ (g) ⇌ $2NH_3$ (g) ΔH = -46.19 kJ A. Increase volume B. Decrease volume C. Increase temperature D. Decrease temperature E. Add N_2 F. Remove N_2
Question Format: Multiple Selection **Cognitive Level of Task:** Retrieval **Type of Task:** Explanation/Interpretation	**Many Choice** Which of the following is/are true? A. It can't be (a) because of Hund's rules B. It can't be (b) because the 3s is getting filled before the 2s is filled C. It can't be (c) because 2p needs to half fill before the first 2p becomes paired D. It is (d) because of Hund's rules E. The question did not need to specify ground state 
Question Format: Free Response **Cognitive Level of Task:** Analysis **Type of Task:** Explanation/Interpretation	**Intermolecular Mixing-Demo** You have 4 compounds: water (H_2O), hexane (C_6H_{14}), iodine (I_2) and potassium permanganate ($KMnO_4$). Two are solids and two are liquids. Based on your observations, where is the water in each of the cylinders? Explain. Cylinder A: potassium permanganate ($KMnO_4$) + Water + Hexane (The purple layer was at the bottom) Cylinder B: iodine (I_2) + Water + Hexane (The purple layer was at the top)
Question Format: Rank **Cognitive Level of Task:** Analysis **Type of Task:** Comparison	**Let's Think** Arrange the following ions from smallest to largest: I^-, Cs^+, Te^{2-}, Ba^{2+} Justify your arrangement
Question Format: Free Response **Cognitive Level of Task:** Analysis **Type of Task:** Calculation/Comparison/Argument	If this dilution was performed with a sample that had 120 ng/L meldonium, would the lab be able to test it? Explain why or why not.
Question Format: Multiple Selection **Cognitive Level of Task:** Analysis **Type of Task:** Interpretation	Which of the following is/are true? A. The charge of the nucleus steadily increases with atomic number B. Zeff always follows the same trend as Z C. For elements in the same group (e.g. Li and Na) Zeff goes up from top to bottom D. For elements in the same row (e.g. Li and O) Zeff goes up from left to right E. The above trends do not change when calculating S as the number of core electrons. 

Question Format: Free Response **Cognitive Level of Task:** Comprehension **Type of Task:** Representation Transformation	**Let's Think** Use the following submicroscopic representation of this process to derive its chemical equation.  Clearly identify reactants, products, and the limiting reactants.
Question Format: Dichotomous **Cognitive Level of Task:** Analysis **Type of Task:** Comparison	**Let's Think** The energy diagrams for two important atmospheric reactions are shown: Which of these reactions is more favored by collision effectiveness? Which of these reactions is more favored by activation energy? Which of these reactions is likely to be fast? A. $N_2\,(g) + O_2\,(g) \rightarrow 2\,NO(g)$ B. $2C\,(s) + O_2\,(g) \rightarrow 2\,CO\,(g)$ 
Question Format: Multiple Selection **Cognitive Level of Task:** Retrieval **Type of Task:** Interpretation	**Learning Catalytics Question** What information can be obtained from point B on the potential energy diagram shown? A. Bond length B. Effective nuclear charge C. Electronegativity D. Bond dissociation Energy 
Question Format: Multiple Selection **Cognitive Level of Task:** Retrieval **Type of Task:** Interpretation	**Many Choice** Select the member of each pair that has the stronger intermolecular forces. CO_2 or OCS (O=C=O or O=C=S) SeO_3 or SO_3 CH_3OCH_3 or $CH_3CH_2CH_3$ A. CO_2 B. OCS C. SeO_3 D. SO_3 E. CH_3OCH_3 F. $CH_3CH_2CH_3$
Question Format: Multiple Choice **Cognitive Level of Task:** Comprehension **Type of Task:** Interpretation	**Let's Think** What can be said about the reaction extent for this process? a) Product-favored b) Reactant-favored c) Product-favored at high T d) Product-favored at low T 
Question Format: Free Response **Cognitive Level of Task:** Analysis **Type of Task:** Model/Inference	**(Whiteboards Out!)** Build H-S Diagram What are the signs of ΔH and ΔS? Is this Reaction PF, RF, or T Dependent? $3\,CO_2\,(g) + 4\,Al\,(s) \leftrightarrow 3\,C\,(s) + 2Al_2O_3\,(s)$
Question Format: Free Response **Cognitive Level of Task:** Comprehension **Type of Task:** Other	**Excerise: Phase Changes & Heat Capacity** Ethanol (C_2H_5O, MW=46.1 g/mol) melts at -114 °C and boils at 78 °C. The enthalpy of fusion of ethanol is 5.02 kJ/mol and its enthalpy of vaporization is 38.56 kJ/mol. The specific heats of solid and liquid ethanol are 0.97 J/g·K and 2.3 J/g·K. How much heat is required to conver 42.0 grams of solid ethanol at -155 °C to ethanol vapor at 78 °C? **ONLY HAD THEM COME UP WITH THE PLAN TO SOLVE!**