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Characterizing Students' Mechanistic Reasoning about London Dispersion Forces

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Supporting Information

ABSTRACT: Characterizing how students construct causal mechanistic explanations for chemical phenomena can provide us with important insights into the ways that students develop understanding of chemistry concepts. Here, we present two qualitative studies of undergraduate general chemistry students' reasoning about the causes of London dispersion forces in nonpolar species such as helium atoms. In the first study, we used semi-structured interviews to examine students' verbal explanations for how and why electrical interactions arise between helium atoms. In the second, we used an online short-answer version of the interview task to examine the prevalence of the drawing and explanation types we observed in student interviews. We present a characterization of students' explanations and drawings in terms of increasing sophistication and demonstrate how it may be used as a model for assessing students' ability to engage in scientific practices such as explanation.

KEYWORDS: *First-Year Undergraduate/General, Chemical Education Research, Noncovalent Interactions, Curriculum, Testing/Assessment*

FEATURE: Chemical Education Research

INTRODUCTION

Understanding the causes and consequences of intermolecular forces (IMFs) is critical to understanding a range of ideas in chemistry from energy changes to physical and chemical properties. The idea that attractive and repulsive interactions within and between molecules influences the ways that molecules behave is central to understanding topics in more advanced chemistry courses (e.g., organic chemistry) and concepts addressed in other STEM courses. Perhaps most notably, the behavior of many biological systems can be explained by considering the ways in which molecules interact, for example enzyme−substrate binding, protein folding, and DNA replication and transcription.

However, prior research in this area suggests that despite explicit instruction in undergraduate-level chemistry courses, many (and in fact *most*) students do not develop a coherent understanding of the nature of IMFs in chemical systems.[1] For example, many students leave the general chemistry sequence without recognizing that intermolecular interactions take place *between* (and not within) small molecules.[1,2] Our prior work in this area has demonstrated that undergraduate general chemistry students can recall definitions of intermolecular forces and give quite reasonable-sounding written discussions of what types of interactions might form between molecules and atoms.[1] However, the same students, when asked to sketch a representation of IMFs to illustrate where they occur, indicated that IMFs (hydrogen bonding, dipole−dipole, or London dispersion forces [LDFs]) are interactions within (rather than between) atoms.[1] Perhaps even more disconcerting is the finding that students who continued into organic chemistry did not significantly change the way they represented IMFs.[1] Given these findings, we should not be surprised when students indicate that bonds break when a substance changes phase or are unable to use mechanistic arrows to predict the ways that molecules interact.[3−5]

There is also reason to believe that, despite instruction, students may fail to understand the *cause* of intermolecular interactions. Prior research has shown that undergraduate chemistry students may attribute atomic−molecular interactions such as covalent bonding to heuristics (e.g., octet rule),[6] teleological interpretations (e.g., atoms "want" to form bonds),[7] or stability,[8] without necessarily invoking the ideas of electrical interactions or how those interactions form. Of the 96 students in our study of how students represent IMFs,[1] only one student indicated that all the types of IMFs were actually interactions between separate molecules. That is, students did not recognize IMFs as examples of the same phenomenon and certainly were unable to articulate that IMFs arise from similar causal mechanisms.

In a related study, we found that students who had been enrolled in a transformed general chemistry course that emphasized interactions as a core idea in chemistry were far more likely to construct representations of IMFs as interactions between molecules than a matched cohort of students from a traditional general chemistry course.[2] While these findings are encouraging, understanding that intermolecular forces occur between molecules is a relatively small component of understanding electrostatic interactions in chemical systems. To develop a robust understanding of structure−property relationships it is also important for students to understand the

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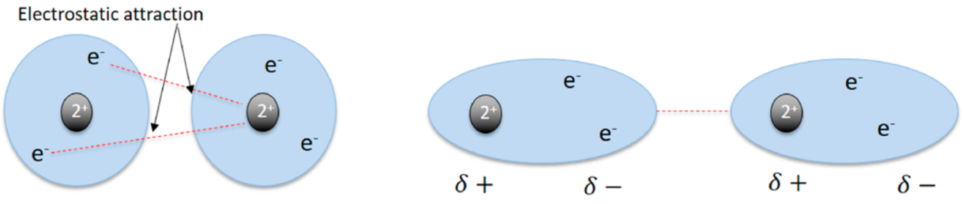

Figure 1. Illustration of London dispersion interaction as formed by two neutral helium atoms.

causal mechanisms of formation of IMFs and the consequences of these interactions. If we are to design targeted instructional interventions to support students' reasoning about these mechanisms, a detailed understanding of the ways students reason about these mechanisms is needed.

■ BACKGROUND

Scientific Explanations and Causal Mechanistic Reasoning

Our overarching goal with this research is to understand how students develop scientific explanations for chemical phenomena. Scientific explanation is one of the eight scientific practices outlined in the *Framework for K-12 Science Education*[9] and is described by the *Framework* as

> *"accounts that link scientific theory with specific observations or phenomena—for example, they explain observed relationships between variables and describe the mechanisms that support cause and effect inferences about them" (page 67).*

Engaging students in the construction of scientific explanations affords them an opportunity to engage (in a scaffolded form) in the practices of science, that is, the activities that scientists engage in as they investigate the natural world.

Scientific explanations may take many forms and may draw on various types of reasoning, ranging from law-based or rule-based reasoning to statistical/probabilistic reasoning to causal mechanistic reasoning.[10] Causal mechanistic explanations offer a unique level of explanatory power across topics and disciplinary contexts in that they provide a way to relate macroscopic phenomena to the underlying factors and relationships that can give rise to a phenomenon.[10,11] A key feature of causal mechanistic explanations is that they move beyond simply identifying relevant causal factors to elaborate relationships and interaction among and between factors and the observed phenomena.[12,13]

In chemistry contexts, explaining emergent chemical phenomena requires that students coordinate information across macroscopic, atomic−molecular, and subatomic levels. Coordinating across scalar levels is a critical skill for undergraduate chemistry students,[14,15,15] yet one that is may be exceedingly difficulty for students. Prior research has shown that students tend to confuse causes and effects across scalar levels.[16,17] Alternately, rather than unpacking the relationship between factors at the atomic−molecular level and relating them to macroscopic phenomena, students may construct non-canonical explanations that attribute macroscopic phenomena to additive properties of atomic−molecular factors, or that simply re-describe the phenomena without discussing specific causal factors.[18]

In this paper we explore how students explain the formation of London dispersion forces in the context of interactions between neutral noble gas atoms. We chose this system not only because it is the simplest way to lead into more complex interactions, but also because LDFs are present in all interactions between neutral species. Our goal is to help students understand that the causal mechanism underlying LDFs can be explained in terms of electrostatic interactions between electron clouds that experience momentary changes in electron distribution. For example, for London dispersion interactions between two neutral helium atoms, students should be able to identify that interactions arise from atomic structure and momentary changes in electron distribution (this process is illustrated in Figure 1). Students should also be able to connect their understanding of these intermolecular interactions to properties of electrical interactions, including the idea that the strength of electrical interactions between atoms varies inversely with distance between interacting species.

Assessment of Causal Reasoning Requires Evidence

Helping students frame scientific questions and construct explanations requires not only appropriately scaffolded instruction, but also appropriate assessment strategies that can provide evidence of the ways that students are making causal connections. Our ultimate goal is to design materials that can not only provide students with the opportunity to tell us what they know, but can also be used to provide feedback to both instructors and students about the level of sophistication of students' responses. Our approach is based on the approach discussed in the NRC report on developing assessments for the Next Generation Science Standards, which is sometimes referred to as construct-centered assessment design.[19] This approach is illustrated in Figure 2.

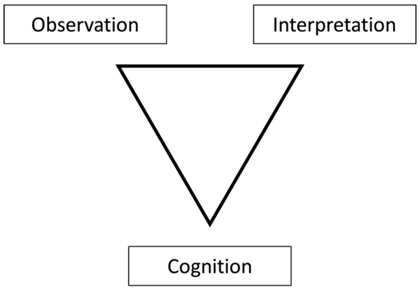

Figure 2. The assessment triangle.

In this approach, we define what we want students to know and do (cognition, or the constructs to be learned) and what observations will be made (the assessment task), and then how those observations will be interpreted. This approach treats assessment as a process of evidentiary argument,[20] where interpretation of the observations is the evidence that will allow us to make an argument about the ways in which students understand the construct at hand. In this approach we draw on both Mislevy's work on evidence-centered design and Wilson's research on construct mapping.[21,22] Rather than identifying whether a student has a correct or incorrect understanding of LDFs (dichotomous), our goal is to characterize the levels of sophistication with which students describe and model LDFs.

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We determine what we would accept as evidence that students have a robust understanding of the construct at hand, and we also delineate the different levels of comprehension that might lead up to this deeper understanding. That is, we are interested in developing a criterion-referenced approach that will eventually help us discern the ways in which students move toward a deeper understanding.

An earlier example of this approach to assessment is the ChemQuery assessment system.[23] Assessment items within the ChemQuery system were developed using Wilson's construct-mapping approach,[22] and items were tested and refined using Rasch modeling to produce a set of "levels" of understanding. The ChemQuery system provides a developmental view of students' understanding that instructors can use to track students' progress toward expert-like thinking across the span of multiple years. However, the criteria for the levels were developed on the basis of expert thinking, meaning that beginning students typically clustered at very low levels, which gives these assessments limited value as a formative assessment within the general chemistry sequence.

In our approach we use student interviews to elicit verbal explanations and sketches of what they think is happening at the molecular level (we refer to these as *drawings*). We then use these student-generated models and explanations to map the ways in which students approach an understanding of the origins and causes of London dispersion forces. We believe this approach will contribute to the design of more nuanced formative assessments that enable instructors to scaffold students' reasoning. Such assessments will enable more detailed descriptions of what students can do with their knowledge, which will in turn shed light on the ways in which different learning environments support students' reasoning.

Research Questions

Specifically, our work addresses the following research questions:

- In what ways do undergraduate chemistry students explain interactions between nonpolar species? (e.g., how do students explain the origins and causes of London dispersion forces?)
- How do students represent, both in words and in pictures, the process by which London dispersion interactions arise?

■ METHODS

Research Design

We report here on two qualitative studies aimed at examining students' understanding of intermolecular forces in simple chemical systems. In the first, we conducted an exploratory qualitative study aimed at characterizing (1) students' explanations of why intermolecular interactions form between neutral atoms and (2) students' molecular-level drawings of what they believe is happening at the molecular level (Study 1). In the second, we used the classification scheme developed in the first study to assess the prevalence of different types of explanations in a larger population of students (Study 2).

Study 1

Participants and Setting. Participants in the first study were undergraduate science and engineering majors enrolled in a first-year general chemistry course at a large research-intensive Midwestern university. Participants were recruited from two sections of an introductory chemistry course, each of which used different curricular approaches. The first section used a transformed curriculum called Chemistry, Life, the Universe and Everything (CLUE)[24] and was taught by the third author. The second course used a traditional approach and a commercially available text.[25] The intent in including participants from both courses was to capture a range of perspectives.

All students were informed of their rights as human subjects, and interview participants signed informed consent forms.

Interview Protocol Design. Our work builds on Williams and Cooper's development and use of the intermolecular forces assessment, or IMFA.[1] Williams and Cooper used the IMFA to assess whether students could construct a drawing to show what three types of intermolecular forces (hydrogen bonding, London dispersion interactions, and dipole−dipole interactions) would look like. While the IMFA also asked students to define in words what terms such as "hydrogen bonding" meant to them, it was not designed to probe students' understanding of how and why these interactions arise. In the studies reported here, we asked students to explain how and *why* intermolecular interactions form in specific contexts—that is, to construct a scientific explanation accounting for the formation of these interactions. We also asked them to sketch a picture to show specifically what might be happening at the molecular level to cause these interactions.

We designed a semi-structured interview protocol based on two of the contexts used in the IMFA: London dispersion forces (in the context of helium atoms) and hydrogen bonding (in the context of water). We used parallel question structures for each interaction type. For the helium context, we asked students to sketch what a helium atom might look like. We then asked them describe what they believed would happen as two helium atoms approached one another from a distance. If a participant indicated that either attractive or repulsive interactions could take place, we would ask them to explain what they meant by "attractive" or "repulsive" interactions and to discuss how the attraction (or repulsion) would arise. If a student struggled with this task, we would follow up with more structured questions that prompted them to talk about what it would look like if the atoms were to attract one another. This part of the interview protocol is included in the Supporting Information.

Pilot Interviews. We piloted the draft interview protocol with two participants using a think-aloud approach. The intent of the pilot interviews was to assess whether tasks were clearly framed and whether the interview protocol would elicit a range of responses, including expert-like responses. The participants were a chemistry graduate student and a sophomore undergraduate biochemistry student who had taken general chemistry the year before. We analyzed the pilot data to examine clarity of interview prompts and the extent to which the questions elicited rich reasoning about students' understanding of intermolecular forces. We determined that the tasks were sufficient for eliciting a range of reasoning. Minor revisions in wording were made prior to the full study.

Study 1 Data Collection. In the fall of 2013, we interviewed 12 first-semester general chemistry students. Ten of these were enrolled in the CLUE course, and two were enrolled in the traditional general chemistry course. Students were interviewed in November, 2−3 weeks before the cumulative final exam. A Livescribe pen was used to record audio and written work.

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Table 1. Overview of the Five Types of Explanations Observed (E1−E5) with Examples from Online Assessment (Study 2)

Type	Explanation features	Description	Example
E5	Canonical electrostatic cause; full mechanism	Student discusses how separation of charge arises due to random fluctuation of electron density **AND** describes formation of an induced dipole	The electrons in one helium atom begin to fluctuate, forming an instantaneous dipole. Consequently, this induces a dipole in the neighboring helium atom. Both atoms now have a temporary positive and a temporary negative region. The opposites of the region are then attracted to one another, and the Van der Waals forces hold them together, though very weakly
E4	Canonical electrostatic cause; partial mechanism	Student explains that separation of charge arises due to random fluctuation of electron density **OR** describes formation of an induced dipole	Atoms move towards each other because of London dispersion forces. London dispersion forces can be explained thus: as one atom moves to another, one half of the atom will become positively charged because it is attracted to the electrons in another **Or** The reason that the atoms are attracted to each other is [that] there is a fluctuation of both of the electron clouds, creating two dipoles, both having a positive and a negative side, and their opposites attracting
E3	Canonical electrostatic cause; little or no evidence of mechanism	Student attributes interaction to dipoles in helium atoms but does not elaborate how charge separation arises	When the helium atoms meet each other the electron distribution will change and the pole of the helium atom will change, and the shape will change too. Positive pole will attract negative pole and will cause the heliums to move towards each other
E2	Non-canonical electrostatic cause; little or no evidence of mechanism	Student attributes interaction to charges of subatomic particles or overall charge of atoms but without the idea of a dipole	I believe that helium atoms move towards each other because of the positive and negative charges within the atom. Since the atoms both have opposite charges, they attract to one another
E1	Non-canonical, non-electrostatic cause; little or no evidence of mechanism	Student attributes cause of interaction to factors other than charge and formation of dipole; may include references to octet rule, stability, or non-specific references to forces	These two helium atoms are resisting each other as they get closer because they do not want to bond. Helium is a noble gas so its outer shell is filled **Or** The forces between the two atoms cause the atoms to move toward each other. Better known as London dispersion forces.

Study 1 Data Analysis. After transcribing all interviews, we used a two-phase analytical approach to examine students' reasoning. The first phase of our approach was informed by McNeill and Krajcik's Claim−Evidence−Reasoning model of a scientific explanation.[26] First, we identified instances in which students made assertions about how or whether species would interact (claim). Then, we identified the information that students used to support their assertion (evidence) and statements in which students elaborated the relationship between evidence and claim (reasoning). Parsing students' explanations according to claim, evidence, and reasoning in this way enabled us to more effectively compare and contrast explanation components within and across cases.

In the second phase of our analysis, we used a constant comparison approach[27] to identify themes in the nature of the ideas present in students' use of evidence and reasoning. Students' drawings were analyzed using an analogous inductive approach. We identified main themes that included five levels of explanations, which we will discuss in the findings section.

Study 1 Reliability. To examine the extent to which the main themes (five levels of explanations for verbal explanations, and four levels for student drawings) could be used to reliably characterize student reasoning, two raters (the first and second authors) independently analyzed text and drawing excerpts from each of the 12 interview transcripts. Initial agreement was 85% for the written explanations passages and 82% for the drawings (Cohen's kappa = 0.810 and 0.768, respectively). After discussion of coding discrepancies, 100% agreement was reached between the two raters.

Study 2

Development of Online Assessment. The goal of the second study was to examine the prevalence of themes in a broader population of students. In the fall of 2013, we designed and piloted an online version of the helium interaction task. The pilot assessment asked students to explain (in writing) how and why helium atoms might interact at a sufficiently low temperature. We administered the assessment to the CLUE general chemistry class in the fall of 2013 using the beSocratic assessment platform[28] as part of a homework assignment ($N = 392$). The homework assignment was graded based on completion only.

Data from the pilot assessment were analyzed using the categories that emerged from our analysis of the interviews. We developed a scoring guide for the text responses based on the themes in reasoning from the interview data and refined our code definitions as we analyzed the online assessment data.

We realized that a significant limitation of the pilot task was that we did not provide an opportunity for students to construct drawings as they had done in the interviews. Additionally, we provided little context for students prior to asking them how and why helium atoms would interact. We revised the pilot task by introducing a simulation showing motion of helium atoms at given temperatures in order to provide a richer context for discussing how and why helium atoms might interact. We also added a drawing task in which we asked students to sketch what might be happening that would cause the helium atoms to move together.

Study 2 Data Collection. We administered the revised task to students enrolled in the fall 2014 CLUE course as part of a homework activity. The course included two sections, one of which was taught by the third author. A total of 717 students completed the assessment.

The final version of the task asked students to watch a simulation[29] of the motion of helium atoms and then to sketch

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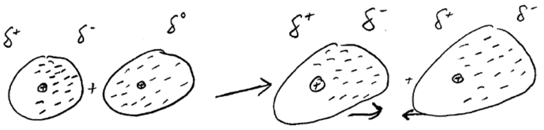
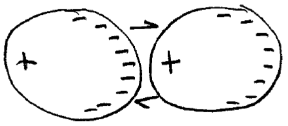
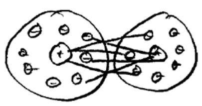
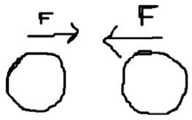
Table 2. Overview of the Four Types of Drawings Observed (D1−D4), with Brief Descriptions and Exemplars from the Fall 2014 Online Assessment

Type	Drawing features	Example
D4	Charges from electrons are shown, as well as separation of charge within atoms; drawing also includes multiple “snapshots” of the system showing how charge separation arises	
D3	Charges from electrons are shown as well as separation of charge within atoms; drawing does *not* include snapshots of the system showing how charge separation arises	
D2	Drawing shows charges of subatomic particles or overall charge of atoms; charge separation within atoms is not shown	
D1	Drawing does not show charge of atoms or subatomic particles; subatomic particles may be represented by spheres or e’s but without information about charge	

a picture and write an explanation for why the helium atoms might move together as shown in the simulation. We hinted that students should consider what might be happening with the electrons and protons of each atom. We included this hint because we assumed that students would already have grasped the basic concept that atoms are composed of protons and electrons. Students received full credit for any attempt at completion of the activity, as was typical for homework assignments in the course. Screenshots of the assessment are available in the Supporting Information.

Study 2 Data Analysis. A random sample was selected from the 717 total online responses using a random number generator in conjunction with the numerical student identifiers assigned by the beSocratic platform. Specifically, we selected 125 responses per lecture section for a total of 250 responses, approximately 30% of the complete data set. We used a deductive approach to analyzing the types of explanations that emerged from the interview data, with themes from Study 1 as analytical categories.

Study 2 Reliability. To assess the reliability of our coding approach, two raters (the second author and a postdoctoral researcher who was not involved with the study) independently coded 60 randomly selected responses from an analogous task administered on a midterm exam (~43% of the total responses). Initial percent agreement between the two raters was 82% for the text responses and 92% for the images, with values of Cohen’s kappa of 0.744 and 0.871, respectively. The two raters discussed discrepancies until 98% agreement was reached (Cohen’s kappa = 0.977).

■ FINDINGS

Study 1

Our participants used a range of ideas to support the claim that helium atoms would experience an attractive interaction, from electrostatic ideas to rules (e.g., octet rule) or teleological notions that atoms “want” to interact. We observed five distinct types of verbal/written explanations (see Tables 1 and 2). These varied in terms of students’ attribution of the cause of the interaction and the extent to which students were able to detail the process by which London dispersion interactions formed. We identified roughly analogous patterns in students’ drawings of this process, though we were only able to discern presence or absence of mechanism (as compared to extent of mechanistic reasoning from verbal explanations). An overview of verbal explanation and drawing types is illustrated in Tables 1 and 2, respectively. We present the qualitative data from which this classification emerged in the following sections.

While we discuss students’ explanations and drawings in terms of a progression toward a more complete and sophisticated causal mechanistic explanation, we do not imply that students progress linearly through these levels. However, we do see a clear shift toward more complex and coherent explanations across Levels E1−E5 that we believe is pedagogically useful.

Level 5 Explanation (E5): Canonical electrostatic cause; full mechanism

We begin our discussion by commenting on what we consider to be a highly sophisticated explanation (for general chemistry students) of how and why London dispersion forces arise. Optimally, general chemistry students would identify that two helium atoms may be drawn together due to an electrostatic attractive force that originates in the arrangements of the charged subatomic particles (electrons and protons). Specifically, one atom may instantaneously experience an uneven distribution of electron density, which leads to a separation of charge (dipole) in that atom. That polar atom may induce a charge on a neighboring atom, which would result in an attractive force between the two atoms.

This type of explanation captures both the cause of intermolecular interactions at the subatomic level (electrons and protons of each atom arranged so as to create a dipole) and the fact that there is an underlying process that leads to the formation of a dipole. In elaborating this process, students must unpack information about the behavior and properties of the entities that cause the interaction. For instance, students must recognize that electrons are in constant motion, that electrons may briefly become unevenly distributed, and that the regions of charge that are formed within a helium atom may exert a force across a distance on a second helium atom. In an ideal causal mechanistic account, each of these ideas would be coordinated to provide a complete and logical sequence of events.

To illustrate this type of complete causal explanation, consider the response provided by Madelyn, a freshman pre-med student. Early in her interview, she had been asked to discuss what she knew about helium atoms and to sketch a picture of what she thought two helium atoms would look like. She drew a representation of a helium atom that indicated the presence of a nucleus and two electrons, and she spontaneously discussed a simulation she recalled from class that showed two helium atoms moving toward one another and forming a stable interaction. She sketched a potential energy curve based on what she recalled about the interaction. When prompted by the interviewer to elaborate on what she thought might be going on that caused the two atoms to move toward one another and interact, Madelyn elaborated as follows:

> **Madelyn:** Two electrons could be on this side causing it to have a dipole. Then that might induce another dipole in this one [draws Figure 3A], and then the positive and negative attract.
>
> **Interviewer:** OK. So now, you mentioned induced dipoles. Can you tell me a little bit more about how you think of that happening?
>
> **Madelyn:** Um, because...an instantaneous dipole is when it just so happens that the electrons are on this side, so there's a slightly negative and slightly positive (drawing) side. And then, because this is slightly positive, it attracts the electrons of this density more towards this side so then it would turn into this [draws Figure 3B].

Madelyn predicted that an individual helium atom could experience an instantaneous dipole due to random shifts in electron density. She reasoned that an instantaneous dipole in one helium atom would induce a dipole in a second helium atom ("it attracts the electrons of this density more towards this side").

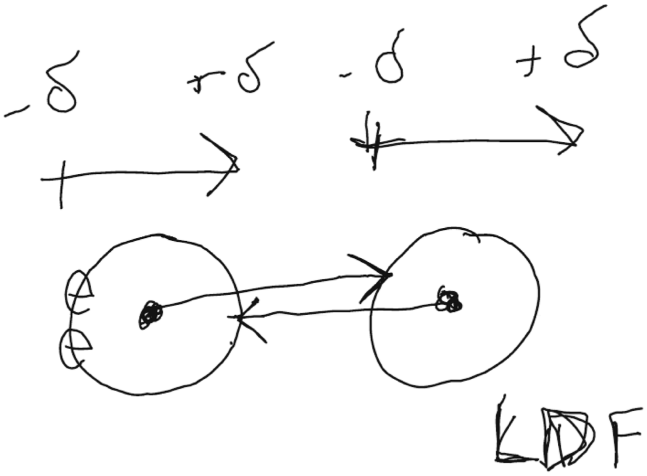


Figure 3. Madelyn's representation of formation of a temporary dipole (A, leftmost atom) and induced dipole (A, rightmost atom). Arrows in panel A represent attraction of the nucleus of the leftmost atom to the electron cloud of the rightmost atom. Panel B illustrates the regions of positive and negative charge in each of the helium atoms (Level D4, electrostatic and mechanistic features).

Madelyn's representation of London dispersion interactions (Figures 3A and B) includes features suggesting both causality, in that she draws electrons and a representation of the nucleus, and mechanism, in that she shows two snapshots of the system, each with different arrangements of electrons and protons. Figure 3A shows a dipole in the leftmost helium atom, but an even distribution of charge for the rightmost atom. Figure 3B shows dipoles in both atoms.

It is important to note that the classification of D4 does not indicate the correctness of students' drawings with reference to canonical depictions of the atoms. Here, Madelyn reversed the arrow she used to show polarity in Figure 3B (typically the vector arrow is drawn pointing in the direction of the negative charge, and in her drawing the vector points to the positive charge). However, this is a notational issue and, overall, her representation addresses both the cause of the interaction (electrons and protons arranged in a dipole) and at least part of the mechanism by which this dipole forms (movement of electrons that results in an uneven distribution of electrons, as she shows in Figure 3B).

Level 4 Explanation (E4): Canonical electrostatic cause; partial mechanism

Other students correctly identified causal factors but constructed explanations with gaps or inconsistencies in the process by which London dispersion interactions form. As an example of this type of reasoning, consider Macayla's reasoning as shown below. When discussing how she thought helium atoms might behave, she noted that helium atoms would form London dispersion interactions, which she described as "instantaneous dipoles that attract and repel one another". The interviewer prompted her to elaborate on how she was thinking about these interactions.

> **Macayla:** With London dispersion forces, they have...instantaneous dipoles that attract and then repel, because they can't form an actual...covalent bond, or actual bond, where they're...sharing electrons.
>
> **Interviewer:** OK. Would you be able to show me more about how you're thinking about these London dispersion forces?
>
> **Macayla:** Sure, OK. So then there's...these would get attracted to each other. Because this one has slightly negative, slightly positive [drawing Figure 4]. And then at some point they get so close that they repel because their electron cloud is getting close to the other electron cloud, which is really close.

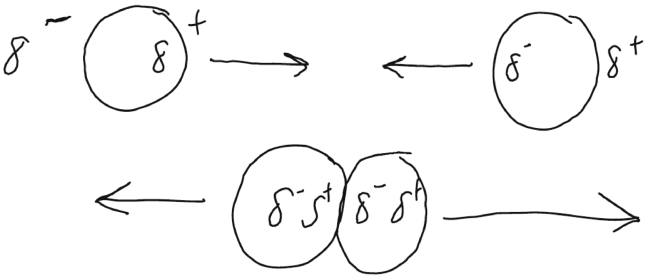


Figure 4. Macayla's drawing of helium atom interaction, with arrows denoting motion of atoms (Level D3, electrostatic features with dipole).

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Macayla recognized that helium atoms interact because of the formation of temporary dipoles which lead to electrostatic interactions between atoms. She depicted this as in Figure 4 by showing a partial positive charge on one side of each atom and a partial negative charge on the other. She also identified that the interaction would become repulsive at close range. In her drawing (Figure 4), she focused on what happens when the atoms approach too closely and begin to repel. She does not show the process by which dipoles are formed, though she describes some aspects of this process verbally; thus, her drawing was classified as Level D3.

When probed further as to her understanding of the process by which the attractive interaction arises, a gap in her reasoning about the process of LDF formation became evident.

> **Interviewer:** So you said that the helium atoms are moving towards one another at some point. What causes them to move towards one another?
> **Macayla:** Umm, their electron cloud is...floppy. So then it moves one way for an instant. And, maybe this electron cloud is on the other side, so then the nucleus is closer to the other atom's electron cloud. And then eventually they are...overlapping. Because it's only...a second, less than that.

Here, Macayla expressed the idea that to cause an interaction, both helium atoms would need to experience a temporary dipole at the same time ("maybe this electron cloud is on the other side"). She did not seem to recognize that a more likely scenario is that a temporary dipole in one atom would induce a dipole in a second. While Macayla identified appropriate causal agents, she did not recognize that simultaneous temporary dipoles are not necessary (and in fact would be highly improbable). This idea that both interacting atoms must experience a temporary dipole at the same time was expressed by two of the 12 interview participants.

Level 3 Explanation (E3): Canonical electrostatic cause; little or no evidence of mechanism

Three interview participants identified that helium atoms could interact via formation of a dipole but were unable to articulate how the charge separation would arise. As an example of this type of reasoning, consider Irene's explanation. Irene identified that helium atoms interact via an electrostatic interaction, but seemed confused as to how that charge separation would arise.

> **Interviewer:** How do you think those two [helium atoms] might interact, if at all?
> **Irene:** Um...they would have the fluctuating dipoles?
> **Interviewer:** OK. Could you show me what you're thinking of?
> **Irene:** [Draws Figure 5] As the atoms approach each other the clouds are kind of fluctuating. So the more relatively positive charge and relatively negative charge are attracting each other.

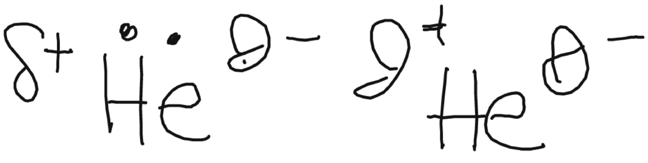

Figure 5. Irene's depiction of positive and negative separation of charge (Level D3, electrostatic features with dipole).

Irene described separation of charge in each atom, noting that there would be a "more relatively positive charge, and relatively negative charge." However, when asked to explain where the positive and negative charges come from, Irene seemed uncertain.

> **Interviewer:** OK. And where do the positive and negative charges come from?
> **Irene:** Um, from the nucleus, and then the um, electrons around the helium.
> **Interviewer:** OK. And you mention that they fluctuate. What's fluctuating? Could you describe that a little bit more?
> **Irene:** Um, they kind of, they go back and forth between, um, I guess, the electrons maybe?

While Irene recognized that helium atoms form dipoles, she was unable to provide a detailed account of the process by which this charge separation occurred. She mentioned that electrons "fluctuate", but seemed unsure of what this term meant. She did not connect the idea of electron fluctuation back to how and why dipoles are formed. Her drawing did not include features that suggested she was thinking about the process by which the dipoles arose, and thus was classified as Level D3.

Two other interview participants also used terminology such as "temporary dipole" and "fluctuation of electron density", but with incorrect or superficial understanding of the terms and their relationship to the process of dipole formation.

Level 2 Explanation (E2): Non-canonical electrostatic cause; little or no evidence of mechanism

Some students were unable to identify that electrical interactions between atoms arise due to specific arrangements of electrons and nuclei in each atom. Yet, they still expressed some understanding of the fact that interactions between helium atoms are electrical in nature.

To illustrate this type of explanation (E2), consider Ryan's discussion of the interaction between two helium atoms. Earlier in his interview, Ryan sketched a representation of two helium atoms that showed two protons and two electrons for each atom. The interviewer then prompted him to consider how the two atoms might interact.

> **Interviewer:** How do you think those two might interact?
> **Ryan:** [Draws line connecting valence electrons as shown in Figure 6A] Um, they might hold on to each other a little bit and make H-2, ah, H, Helium gas? He_2?
> **Interviewer:** OK.
> **Ryan:** Well I thought...no. I don't know how exactly those act together.
> **Interviewer:** I see that you've drawn a line between the two. Could you tell me more about that? What's going on there?
> **Ryan:** Um, it was kind of just a representation of a, some sort of...like a, not dipole−dipole. It's a London dispersion bond.

Interestingly, Ryan was able to name correctly the type of interaction that would form between neutral helium atoms (i.e., London dispersion interaction). However, beyond the recognition that electrons were involved in this interaction (as indicated by his drawing of a connection between electrons on adjacent atoms in Figure 6A), Ryan admitted he was unsure of what this interaction entailed. When prompted to elaborate on

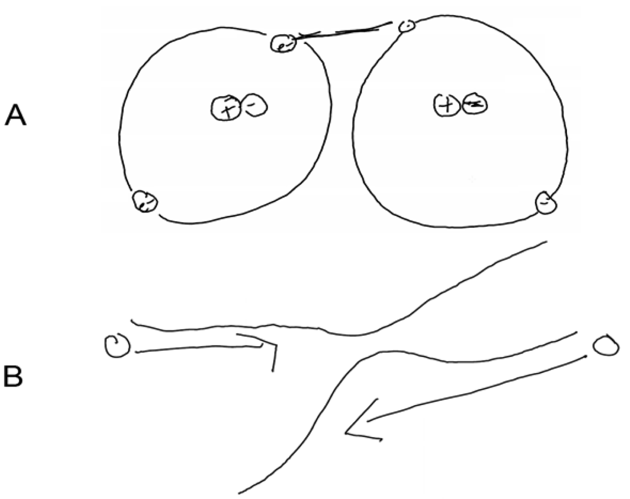

Figure 6. Ryan's depiction of how an attractive interaction would influence the trajectory of adjacent helium atoms (Level D2, electrostatic features without dipole).

his earlier mention of the particles "holding on" to one another, he discussed how the trajectories of gas-phase helium atoms might be influenced by an attractive interaction (Figure 6B).

As a rationale for why the atoms might be attracted to one another, Ryan discussed how the electrons from one atom might be simultaneously attracted to nuclei of both atoms.

> **Interviewer:** What's going on with the protons and electrons when they do that [attract]?
>
> **Ryan:** This proton is holding onto its electrons. And then let's see, it has this other electron coming who's like all positive and negative and attracted to that [nucleus from first helium atom]. But then this one [second helium atom] is also pulling on that electron at this same time, but it has a stronger connection to that one [second helium atom] because it's closer to that one than that one would be.

Ryan correctly identified that the strength of an electrical interaction would be inversely related to the distance between particles and used this idea to reason about the relative magnitudes of interaction between electrons and the two helium nuclei. This idea that the strength of electrical interaction is inversely proportional to the distance between interacting species was identified by students with all levels of explanations.

While Ryan recognized that an electron could be simultaneously attracted to two separate nuclei, he did not seem to recognize that for the interaction between atoms to be significant enough to affect the trajectory of atoms there would need to be a specific arrangement of electrons and protons (i.e., a dipole). Ryan's explanation lacked the idea of a dipole. Not surprisingly, he did not discuss the process by which a dipole would be formed.

While Ryan used some correct ideas about the nature of electrical interactions, (i.e., that strength of interaction is inversely proportional to distance between particles), he also used some electrostatic ideas imprecisely or incorrectly, suggesting difficulties in understanding the nature of electrical interactions. For instance, earlier in his interview, he indicated that an interaction would form between two adjacent helium atoms via linking of electrons. Later, he noted of the helium atom that "it has this other electron coming who's like all positive and negative and attracted to that." Though Ryan recognized that protons and electrons are charged, he seemed unable to articulate the relationship between the arrangement of subatomic particles and the attractive force between atoms. Overall, Ryan's reasoning suggests a fragmented understanding of electrical interactions, their relationship to subatomic structure, and their role in interactions between atoms.

Level 1 Explanation (E1): Non-canonical, non-electrostatic cause; little or no evidence of mechanism

The last type of explanation we observed involved students' use of non-electrostatic ideas as explanations for why helium atoms might be attracted. Such non-electrostatic ideas included the notions of "stability" or the octet rule as driving atoms to share electrons. In the online assessment, we also identified students who made assertions that a "force" would draw two atoms together but provided no additional detail regarding the nature of the force: for instance, "the helium atoms have London dispersion forces in between; they are being attracted towards each other by a force."

We observed only one instance of this type of explanation in the semi-structured interviews, but more in the online assessment. Students who gave this type of explanation often expressed a belief that helium atoms would form a covalent bond. For example, one interview participant, Devon, believed that helium atoms would come together to form an He_2 molecule. However, to form this molecule, helium atoms would first need to overcome a repulsive interaction.

> **Devon:** So, as the two helium atoms approach they're going to repel. They're going to...not want to interact. But then once they get over those repulsive forces, then they're gonna form a molecule of helium.
>
> **Interviewer:** OK. So you mentioned repelling. Can you tell me a bit more about that?
>
> **Devon:** Well they're both...they have the same charge. And opposite charges attract, so...they have the same charge. They're gonna want to repel.

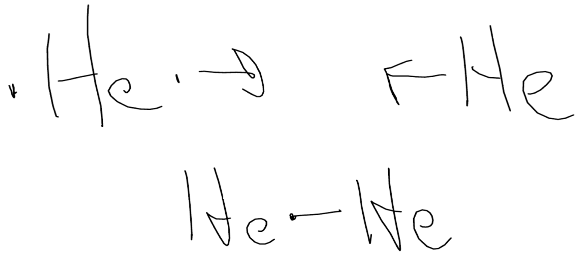

Figure 7. Devon's depiction of interaction between helium atoms (Level D1, no electrostatic features).

Devon predicted that helium atoms would initially repel rather than attract based on the fact that each helium atom has two valence electrons (shown in Figure 7), and thus would have the same net charge. This initial portion of Devon's reasoning is, in fact, electrostatic and is aligned with Level E2 reasoning.

However, Devon went on to indicate that the repulsive interaction would be overcome and the helium atoms would be drawn together to form He_2. With respect to his explanation of why "drawing together" would occur, Devon mentioned stability, but with some uncertainty related to the stability of the molecule relative to separated helium atoms.

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> **Interviewer:** OK. So, you also drew arrows that sort of point this way. What makes them come together to form a molecule like that?
>
> **Devon:** Um, I'd say stability, but they're already pretty stable, because they're in the noble gases. So, um...

Later in his interview, Devon indicated that he was, in fact, familiar with London dispersion interactions. However, he seemed to have a misconception about the nature of the interaction. Specifically, he seemed to believe that intermolecular forces take place between molecules only (and not atoms).

> **Devon:** Well, they're [London dispersion forces] only present between two molecules. So, if you just had two atoms of hydrogen, let's say for example, it wouldn't be present because there's atoms. But if we had, like, two molecules of water, it'd be present. Like, the force would be present between those two because it has to do with the electrons of one molecule being attracted towards the nucleus of another molecule.

He later commented that he knew that he did not understand the cause or mechanism by which London dispersion interactions arise.

> **Devon:** So I guess you could say this is like a problem I have, with...learning and how I've been conditioned to learn, because...I'm not trying to make excuses, but, like, throughout high school...the generally accepted thing is to, like, go through something, memorize it, be tested on it, and then kind of push it off.

Notably, Devon referenced his high school learning experience as part of what he believed conditioned him to focus on facts and rote memory in his learning of chemistry.

In summary, Devon seemed to hold a misconception about the nature of London dispersion interactions in that he believed that they formed only between molecules. When discussing interactions between helium atoms he was unable to relate the interactions to subatomic structure or electrical forces, suggesting little understanding of how different types of interactions are formed. We argue that failing to recognize that interactions between atoms and molecules are electrostatic makes it exceedingly difficult for students to see similarities and differences across these types of interactions.

Study 2 Findings

As noted earlier, our ultimate goal is to develop assessment tasks that elicit evidence of the level of sophistication of student explanations. In this section we present the analysis of students' written explanations and drawings in response to the prompt "Draw a molecular-level picture of what happens when two atoms of He approach each other. Use the picture to help you explain why the two atoms are attracted." We analyzed students' drawings and written explanations using the categories developed from the student interviews. We also added an additional category (D0) to denote drawings in which students drew a representation with no discernible features relating to helium atoms or interactions (8 out of 250 responses).

The frequency of responses in each of the drawing and text categories is shown in Figures 8 and 9. Examples of each type of response are shown in Tables 1 and 2.

Figures 8 and 9 illustrate that relatively few students included information about the mechanism by which helium atoms interact in either their written explanation or their drawings. Most students did, however, include some electrostatic features in either their explanation or their drawing. As shown in Figure 8, the most prevalent type of written explanation was Level E2, which accounted for 43% of student responses. E2 explanations identified the cause of helium atom interactions as relating to electrostatic phenomena, but did not articulate a mechanism by which the dispersion of charge arises. We believe this type of explanation may have been especially prevalent because students who are still learning about London dispersion forces appear to understand that they originate from the charges of subatomic particles, but are not yet able to describe how a dipole arises from a neutral species.

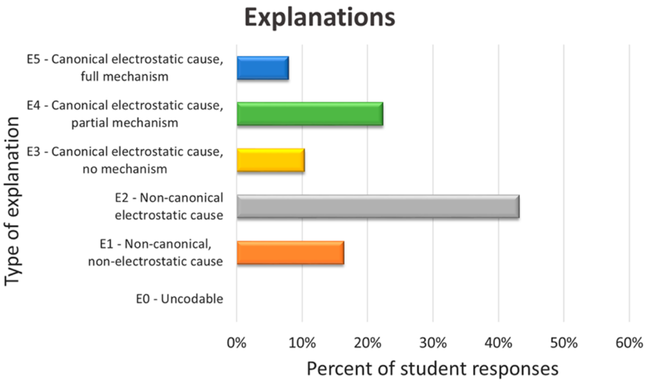


Figure 8. Frequency of explanation types for formative assessment task administered in beSocratic; $N = 250$.

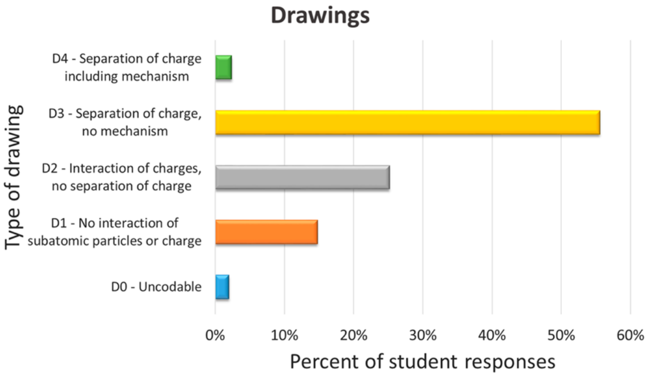


Figure 9. Frequency of drawing types for formative assessment task administered in beSocratic; $N = 250$.

While 41% of students described the presence of a dipole in their written explanations (Levels E3–E5), 58% showed the presence of a dipole within each helium atom dipoles in their drawings (Levels D3, D4). One possible explanation for this observation is that students may have been familiar with representations such as that shown in Figure 3B, where separation of charge within an atom is represented using partial positives and partial negatives. This type of representation had been used in discussions of polarity and intermolecular interaction in the CLUE lectures. The lower prevalence of the idea of a dipole in students' written explanations may suggest that students did not necessarily understand what that representation meant or how to explain it.

To further examine the correspondence between explanation and drawing levels, we constructed the Sankey diagram in Figure 10. We collapsed our codes into three broader categories: non-electrostatic explanations and drawings, electrostatic explanations and drawings, and causal mechanistic

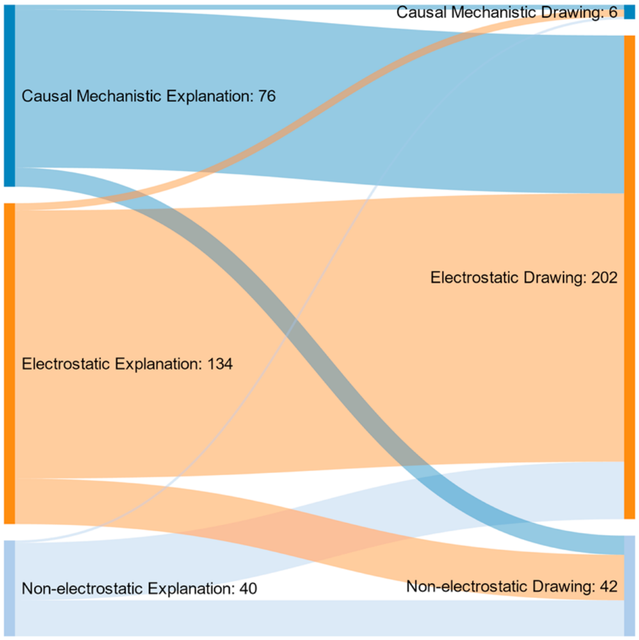


Figure 10. Sankey diagram showing prevalence of non-electrostatic, electrostatic, and causal mechanistic explanations (left) and drawing (right). $N = 250$.

explanations and drawings. The non-electrostatic category included explanations and drawing characterized by non-electrostatic features only (Levels E0, E1, D0, D1). The second category, electrostatic, included explanations and drawing with electrostatic features but no mechanistic details (Levels E2, E3, D2, D3). Lastly, the causal mechanistic category included explanations and drawing that included both electrostatic features and features representing the mechanism by which London dispersion interactions are formed (Levels E4, E5, D4).

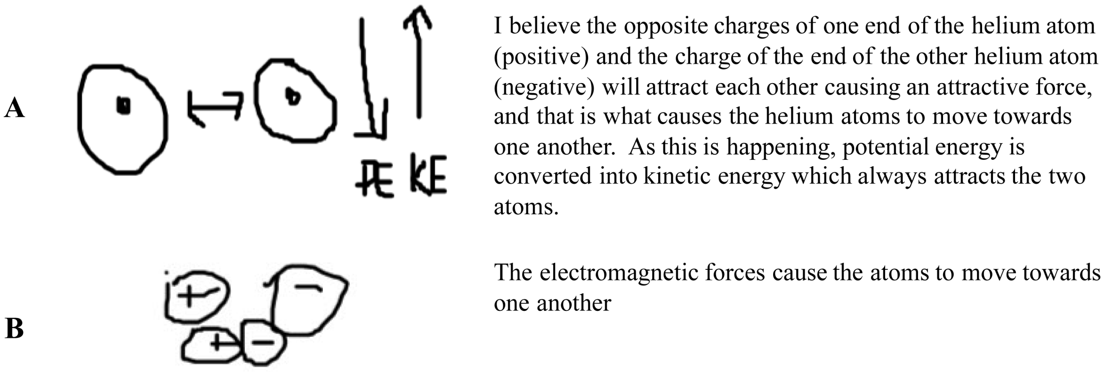
Figure 10 illustrates that the overwhelming majority of students who constructed electrostatic explanations also showed electrostatic features in their drawing. However, of the students who discussed the mechanism by which a dipole would form in their explanation ($N = 76$), only a small fraction included mechanistic features in their drawing. We believe this observation is most likely an artifact of the assessment prompt in that we provided only one box for students' drawings, making it challenging for them to include detail about the sequence of steps by which dipoles arose. The prompt was not explicit that students should show the *process* by which an interaction arises, and thus this may be a limitation of the assessment task.

From Figure 10 we can also see there were a number of instances in which students constructed a non-electrostatic drawing and an electrostatic explanation (and vice versa). Of the students who constructed non-electrostatic explanations, 60% (24/40) included some electrostatic features in their drawing. Of the students who gave electrostatic explanations, 14% constructed non-electrostatic drawings. To illustrate these types of responses, Figure 11A shows an example of one student's Level D1 drawing and Level E3 explanation. Her explanation seems to reference an uneven charge distribution within an atom, though it does not indicate how that charge distribution arises or how specifically subatomic particles contribute to a charge separation. She also discussed the impact the interaction would have on the potential and kinetic energy of the particles (which was not addressed by the question prompt). Looking at both her drawing and representation together suggests either that she was overly focused on the idea of potential energy or that she may not have fully understood what "charge separation" means in this context.

Figure 11B illustrates a student response that included a Level D2 drawing and a Level E1 explanation. The student's drawing included charges within atoms but suggested that helium atoms possess a net charge. The student's explanation for why helium atoms would be drawn together included the superficial use of the term "electromagnetic forces", without elaboration of what this term means or how an electrical interaction would arise. We interpret this drawing and explanation together as suggesting limited understanding of the nature of electromagnetic forces and how the structure of helium atoms contributes to an electrical interaction between atoms.

■ LIMITATIONS

The online assessment data presented here are taken from a low-stakes assessment (a homework activity on beSocratic) that was graded only for completion, not correctness. It may well be that results from high-stakes assessments will provide different levels of response as students may have more motivation to articulate their reasoning clearly. However, we believe that our approach is generalizable enough that others may use it as a



I believe the opposite charges of one end of the helium atom (positive) and the charge of the end of the other helium atom (negative) will attract each other causing an attractive force, and that is what causes the helium atoms to move towards one another. As this is happening, potential energy is converted into kinetic energy which always attracts the two atoms.

The electromagnetic forces cause the atoms to move towards one another

Figure 11. (A) A Level D1 drawing (non-electrostatic) and a Level E3 explanation (electrostatic with dipole). (B) A Level D2 drawing (electrostatic) and Level E1 explanation (non-electrostatic).

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scoring guide to investigate how students think about London dispersions forces.

Our findings suggest that without explicit prompting, many students may not think of interactions in terms of atomic–molecular structure and the mechanisms by which interactions are formed. The framing of the question prompts used in this study, notably that the prompt did not explicitly ask students to consider the process by which dipoles form, may have influenced this finding. In a forthcoming study, we further explore influences of question structure on students' reasoning on the formative assessment tasks by providing explicit prompts for the mechanism component, specifically by asking students to draw multiple pictures of the process by which London dispersion forces arise.

While we do see a general pattern of progression toward greater sophistication as students move from lower levels (E1, D1) toward higher levels (E5, D4), students may not progress linearly through these levels as their understanding grows. Further research to examine individual students' trajectories as they progress through chemistry courses is thus warranted.

■ CONCLUSIONS

The characterization of students' reasoning from the interview portion of our study provides insight as to how students develop more expert-like thinking about atomic–molecular interactions. Notably, this characterization highlights key transitions in students' reasoning about interactions between atoms. First, we observed a transition that we believe represents a shift from non-electrostatic reasoning (Level E1) toward explanations that appeal to electrostatic features in the structure of helium atoms (Level E2). Between Levels E3 and E4, we see a transition away from a simple recognition of the agents involved in the interaction (arrangement of subatomic particles that contributed to a dipole) and toward recognition of the process by which that specific arrangement of electrons and protons arises. In contrast to E4 explanations, which gave partial details regarding the mechanism by which an LDF forms, E5 explanations described a complete sequence of events leading to the formation of an LDF interaction between helium atoms.

We used the characterizations developed from semi-structured interviews to examine responses from a larger population of students. We found that, immediately after instruction, a majority of students explained interactions between helium atoms at Level E2 or E3, suggesting a recognition of the cause of helium atom interactions as electrostatic in nature. However, most students provided limited detail as to the mechanism by which electrical interactions arise between neutral atoms. Since understanding how and why these interactions arise is critical for understanding a range of chemistry content, from phase changes to non-ideal gas behavior and solubility, we therefore suggest that students may require some instructional scaffolding if they are to develop the ability to articulate this type of explanation.

Our findings suggest that it is important to examine student-constructed drawings representing a phenomenon as well as their verbal/written explanations. We observed that about one-third of our participants in Study 2 were able to draw diagrams that were more sophisticated than their written explanation according to our levels of classification. It is important to note that there are multiple factors that contribute to students' ability to construct a robust explanation in this context including their understanding of atomic structure, their ability to articulate their thinking in writing, and their understanding of the nature of scientific explanations. Our findings may suggest that some students had difficulty articulating their thinking even though they were able to construct a drawing that highlighted relevant causal aspects of the system. As such, assessment questions that ask for only one modality may miss aspects of student understanding. However, we believe that when drawing and explanation are examined together these characterizations can provide useful insight into students' specific reasoning difficulties.

■ IMPLICATIONS

Using the levels of reasoning that emerged from our analysis of structured interviews, we developed a scoring guide that enabled us to characterize large numbers of student drawings of London dispersion forces. An analogous approach may allow instructors to use information from similar assessment tasks to refine and redesign curriculum materials to better support students in constructing causal mechanistic explanations of chemical phenomena.

For instance, in our work with the CLUE curriculum, we noticed that many students initially gave non-electrostatic responses following instruction, we have redesigned formative assessments to explicitly give students cues as to the nature of reasoning we are interested in (e.g., electrostatic). To help students think about the mechanism of the interaction we have redesigned the drawing task to require that students sketch pictures of atoms at various points as they move toward one another. We have also begun using student drawings and responses from the homework (formative tasks) as a starting point for in-class discussions of the strengths and opportunities for improvement in students' explanations. We will report on the effect of these instructional shifts in a later publication, but is reasonable to believe that such targeted instructional scaffolds can have a significant impact on students' understanding. In our ongoing work, we are examining students' reasoning about related interactions, such as hydrogen bonding interactions, and how students' understanding of such interactions contributes to their reasoning about chemical phenomena such as phase change and solvation.

We argue that our characterization of students' explanations of how and why helium atoms interact has the potential to help instructors assess students reasoning in a way that goes beyond assessing whether students recognize different types of interactions. We qualify this claim by noting that further research is needed to design assessments that are valid and reliable for different populations of students as would be appropriate for programmatic assessment or supporting claims about how students' knowledge progresses under various instructional settings. However, as formative assessments for learning, that is, for giving students practice in engaging in rich scientific practices such as constructing models and using them to support causal mechanistic explanations, these characterizations are a useful first step.

■ ASSOCIATED CONTENT

Ⓢ Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.6b00298.

> The semi-structured interview questions that were used in this study as well as screenshots from the online assessments (PDF, DOCX)

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Notes

The authors declare no competing financial interest.

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