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Students' Approaches to Determining the Location of Intermolecular Force between Two Distinct Molecules

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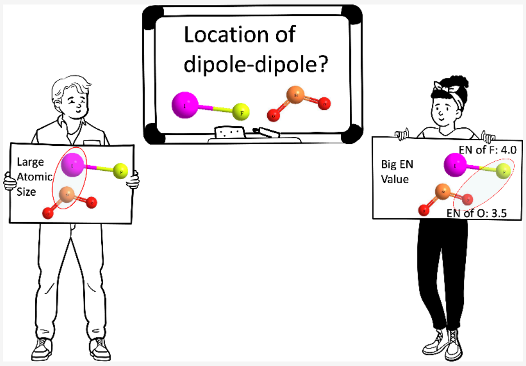
ABSTRACT: Studies investigating chemistry students' understanding of intermolecular forces have listed alternative conceptions; however, there is a call to investigate why students might have these alternative conceptions. This study describes how second semester general chemistry students predict the location of dipole–dipole forces between two molecules from a resource activation perspective. During interviews, 18 students were asked to describe the location of forces between four pairs of molecules. Students relied on one or more of the following approaches in determining location: (1) attraction between opposite charges, (2) electronegativity differences, (3) biggest electronegativity values, (4) largest atomic size, and (5) molecular shape. Each student's approach is characterized by the resources being activated and, in particular, students' use of electronegativity. Students' use of electronegativity varied, including comparing electronegativity values between unbonded atoms within a molecule and between atoms present on different molecules. The findings suggest future research directions and teaching implications that could improve students' understanding of intermolecular forces including the explicit integration and assessment of the concepts of electronegativity and intermolecular forces.



KEYWORDS: *Chemical Education Research, General Chemistry*

BACKGROUND

Intermolecular forces are a foundational topic in the college chemistry learning sequence.[1] It rationalizes how chemicals different from each other interact, such as solvents in a reaction or the structure of biological macromolecules.[2] High school and general chemistry students struggle in understanding how intermolecular forces occur and where they occur; for example, it has been shown that students may identify intermolecular forces as within molecules[3−5] and that this concept can continue into organic chemistry.[6−8] Other studies have explored how students translate intermolecular force strength into predictions of physical properties, finding students also treat intermolecular forces as within molecules.[3,9]

Cooper and colleagues[8] conducted a recent investigation on the prevalence of students' conceptions regarding the location of intermolecular forces. In this work, they administered an assessment that asked students "what is your current understanding" of each intermolecular force and to draw and label the intermolecular forces present among a set of three ethanol molecules. In students' drawings, 61% drew dipole–dipole within a molecule while only 11% drew it between molecules. In contrast, the same students' written responses on their understanding of intermolecular forces had 49% explicitly describe dipole–dipole as between molecules. The authors were not able to detail why the different prompts led to differing accuracy in describing the location but did describe the written responses as somewhat superficial and difficult to interpret owing to ambiguity of chemical terms (e.g., conflating the terms atom and molecule). The inconsistencies between drawing and text in student conceptions of locations were most prevalent when assigning dipole–dipole as opposed to other intermolecular forces, and the authors hypothesized that students may have been utilizing a learned definition of dipole–dipole that specifies the location as *between* molecules. The results of this study highlight widespread student challenges in describing the location of intermolecular forces, including some success in students' writing about dipole–dipole which evidently did not carry over into their drawings.

The current study seeks to understanding why students are challenged in determining the location of dipole–dipole forces. In so doing, this study matches calls in the literature to assess students' use of concepts to predict intermolecular forces.[8,10] Building on past work that relates student understanding of electronegativity to bond and molecular polarity,[6,11−13] this study will expand the scope to consider how students'

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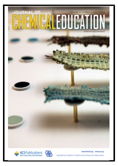

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conceptions influence the prediction of the location of dipole–dipole forces. To date, no studies could be located that described how students use electronegativity values to make predictions about the location of dipole–dipole forces, a gap that the current study seeks to address. Predicting the location of dipole–dipole forces acting between the molecules is essential for chemistry students, since similar skills are needed in biochemistry to understand the role of noncovalent interactions in protein folding. Additionally, the process of predicting the location of dipole–dipole forces includes assigning locations of molecular polarity, which is an essential skill in predicting reaction mechanisms which are common to organic chemistry.

Past studies in chemistry education examine students' abilities to identify the type or location of intermolecular forces that occur between two identical molecules (e.g., H_2O to another H_2O).[8,9,14] However, there is evidence that students apply the concept of electronegativity freely, and the varying applications of electronegativity may not manifest when students examine two identical molecules. For example, studies have shown that students attribute bond polarity to absolute electronegativity values, whether atoms were connected or not, leading to a conclusion that particular atoms (e.g., hydrogen) will always be nonpolar.[15] It is assumed that students will demonstrate more variation in their use of electronegativity values, bond polarity, and molecular polarity when given two distinct molecules (e.g., H_2O and SO_2) than when given two identical molecules, owing to the higher degrees of freedom in the two distinct molecule system. That is, distinct molecules provide more variations in how electronegativity values might be employed including absolute values or comparing values across nonbonded atoms and that distinct molecules will provide a clearer indication when these variations are employed. Further, modeling the interactions between distinct molecules has broad applicability to systems students will later encounter including solvation and substitution reactions. Thus, as this study seeks to determine the range of variations among students' processes, this study will depart from the literature by purposely investigating students' perceptions of interactions between distinct molecule pairs.

Several studies show pedagogical interventions to teach intermolecular forces at the college level, such as inquiry-based,[16] through a structural database,[17] using argumentation with tactile models,[13,18] card games, and lab activities.[19] Concept maps have been designed to expose students' gap in understanding the role of intermolecular forces in chemical bonding.[6,20] The findings from this study may further inform these efforts to support students learning this topic by describing the salient topics students bring forth related to intermolecular forces.

Rationale

The research literature demonstrates that students struggle with identifying the location for intermolecular forces and students use electronegativity values in noncanonical ways. Combined, these points suggest there is a need to investigate why students struggle approaching intermolecular forces by honing in on the use of electronegativity. This study therefore investigates students' approaches to predicting the location of dipole–dipole forces including their utilization of electronegativity. Dipole–dipole was the chosen intermolecular force for this study because of student struggles documented in the literature[8] and the reliance on electronegativity to predict bond dipoles. This study is therefore guided by the following research question: *In what ways do general chemistry students approach predicting the location of dipole–dipole forces between molecules?*

Analytical Framework

As the goal of this study is to describe the variety of ways students describe identifying the location of dipole–dipole forces, this study follows the analytic approach of phenomenography.[21] Phenomenography seeks to describe the variation in experiences across a sample and does not seek to develop an underlying essence common across the experiences.[22] It is also recognized that this approach discovers a limited number of ways that participants experience a phenomenon and does not claim to uncover all the ways a phenomenon can be experienced.[22] For the purposes of this study, the phenomenon is operationalized here as the task of identifying the location of dipole–dipole forces between two distinct molecules. This framework was chosen as, first, the way students learn is an internal relationship between themselves and the experience of the phenomenon.[23] Since this relationship could change from student to student and across molecules and representations, this study sought to explore students' conceptions across a set of molecules and using different representations. Second, students' understanding of intermolecular forces is less likely to be constructed in isolation,[24] and because electronegativity is essential to demonstrating intermolecular forces, there is an assumption here that students' conceptions of electronegativity have the potential to influence conceptions of intermolecular forces. Therefore, the phenomenography framework will help in bridging how students relate their concepts of electronegativity to their concepts of intermolecular forces.

Theoretical Framework

Resource activation framework takes into account the social constructivist point of view that knowledge is constructed by the learner and is dependent on their environment.[25] Since the current study makes use of phenomenography, the learner can detail pieces of their knowledge that were cued to them during the interview and these pieces could be the different resources that are activated when asked a question. Resources do not occur in isolation (similar to knowledge in pieces[26]); rather, activation of a particular resource could cue activating another.[27] Thus, the resource perspectives when used with interviews can uncover students' finer-grained resources that are context-specific.[28]

Resources are neither right nor wrong. The learner's goal is to sift through the resources and pick one that fits the context.[29] A particular resource might be misleading depending on the context. For example, solid is denser than liquid, but in the case of water, ice floats instead of sinking in the water. Here, the resource "solid is denser than liquid" is applicable; except in this context, another resource needs to be activated to describe the context of water. Just because the resource "solid is denser in liquid" was not sufficient in the context of water does not render the resource useless, as in other contexts it might be useful. Thus, the context decides whether a resource is productive.[27] Since resource activation is seen with the social-constructivist framework, resources can be seen as building blocks, and when multiple resources are linked or built upon each other, a thorough understanding of the task at hand could be uncovered. Thus, this study makes use of phenomenography to detail the variations in student processes and resource frameworks to offer an explanation for these variations.

■ METHODS

Participants

The study took place at a research-intensive university in the southeast region of the United States. The participants were recruited from second semester general chemistry. At the time of the study, there were 7 classes of second semester general chemistry with 1369 students enrolled. These seven classes were coordinated; that is, they were taught by different instructors, but each class followed an agreed upon syllabus, common homework assignments, and in-term and final exams. The institutional review board approved the procedures for this study. At the time of the interview, students had covered bond polarity and molecular polarity in first semester general chemistry and intermolecular forces in second semester general chemistry. Recruitment messages went out to batches of 50 students randomly selected via messaging through the students' learning management software. After each round of sending messages, interviews were conducted, and another round was sent out if the researchers continued to observe participants using approaches deemed novel from past interviews. Following the interviews after the third round of sending out recruitment messages, the researchers reviewing the data believed participants' responses were matching previously observed responses. This resulted in 18 interviews, matching the general sample size guidelines given for phenomenographic studies.[22] After each interview, the interviewer wrote a summary and shared highlights with the other researchers, and through these discussions, the researchers decided that they were observing similar ways of how students were approaching the given task; thus, it was judged unlikely that recruiting more students would readily lead to observing new processes.

The time point chosen for recruiting and conducting the interviews was after the first term exam in the second semester general chemistry course, which follows instructional coverage of intermolecular forces and marks the first time this topic was formally assessed. The exams are multiple choice and questions from the exam that dealt with intermolecular forces involved interactions between molecules with the same identity. Informed consent was obtained from each participant, and participants were each compensated with a $25 gift card for completing the interview.

Data Collection

In-person semistructured interviews were conducted for this study. Each interview was 30 to 60 min long. Participants were given the prompts on an iPad and could use an electronic pencil to draw on the screen, as drawings have been shown to demonstrate unique responses when describing intermolecular forces.[8] The interviews were audio recorded to capture participants' explanations, and screen captures of students' sketches recorded participants' drawings. An interview included one ice breaker question and two sections about chemistry (see the Supporting Information for full interview protocol). The focus of this study will be the second section, prompts 2a through 2d that asked students to predict the location of the strongest intermolecular force (dipole−dipole) in each of the four sets, asked one at a time, where each set contained two distinct molecules. The molecular representation (chemical formula, Lewis dot structure, ball and stick, and space filling) changed for each set.

The original intent of this study was to investigate the impact of representations on students' selection of location of dipole−dipole forces. Through an exploration of the data, an apparent avenue of inquiry arose by focusing on variations in students' processes when determining the location of dipole−dipole forces. This study focused on students' processes when prompted to consider the role of electronegativity values in the task. The data showed variation in ways students approached the task, including instances where students did not utilize electronegativity values despite the prompting. These variations are the focus of the current study and inform how students construct an understanding of dipole−dipole forces. The intent is to examine the impact of representations in a future study. Since the aim of the current study is to describe the range of variations in students' processes, it is worth noting that changing the molecular representations students see may cue variations not observed when representations are consistent, as past work has shown that representations may cue students to different features.[30]

Two versions of the interview were created. Each version used the same set of molecules in the same order but differed in the order of molecular representations as shown in Figure 1.

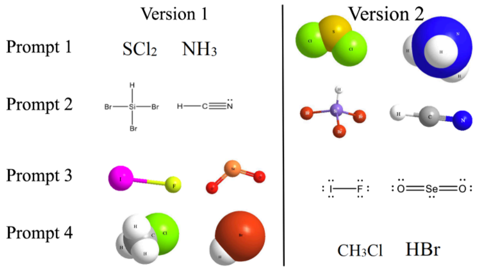


Figure 1. Representations of pairs of molecules given to students during interview versions 1 and 2.

Nine interviews were conducted with each version. The interviewer would ask the same question for each set: *Imagine the following two molecules are in a solution next to each other. The strongest intermolecular force between them is dipole dipole. Identify the pair(s) of atoms where the strongest intermolecular force would occur? Draw a dotted line connecting these atoms.* Students were given the following pairs in order: (i) sulfur dichloride and ammonia, (ii) tribromosilane and hydrogen cyanide, (iii) iodine monofluoride and selenium dioxide, and (iv) chloromethane and hydrogen bromide. The pairs of molecules are shown in Figure 1. Electronegativity values for each atom in the molecules were provided to the students. This was done to reduce the time during the interview to recall or refer to an electronegativity chart for values of each atom. Each interview was conducted by one of the first two authors.

It is important to draw attention to the use of the "pair(s) of atoms" direction in the interview prompt. Canonically, the source of intermolecular forces within molecules with multiple bond dipoles can be in an interatom region (e.g., the positive dipole in NH_3 is situated among the three H's). Some of the representations used do not portray molecular geometry explicitly (see Figure 1), and therefore, participants would not be able to diagram an intermolecular force into an interatom region with the representations provided. The pair of atoms direction serves as a simplification where

Table 1. Summary of Approaches Used in Determining Dipole−Dipole Location

Approach	Basis for Selecting Location of Interaction	Description of Approach	Predicted Location
1A	Opposite charges attract	Dipoles based on electronegativity differences among bonded atoms	*Inter*molecular or *Intra*molecular
1B		Dipoles based on electronegativity differences between atoms in different molecules	*Inter*molecular
1C		Dipoles based on electronegativity differences between unbonded atoms within one molecule	*Inter*molecular
2A	Differences in electronegativity	Dipole−dipole between atoms whose electronegativity values differ by more than 0.5	*Inter*molecular or *Intra*molecular
2B		Dipole−dipole between atoms that have the largest electronegativity difference	*Inter*molecular
3	Size of electronegativity values	Dipole−dipole between atoms with the largest electronegativity values	*Inter*molecular
4	Atomic size	Dipole−dipole between atoms with the largest atomic size	*Inter*molecular
5	Molecular shape	Dipole−dipole within molecule with bent shape	*Intra*molecular

intermolecular forces can be attributed to atoms that contribute to the molecular dipole. This simplification is used in introductory chemistry textbooks when diagramming intermolecular forces, including the textbook used at the research setting.[31−34] This direction may influence students away from invoking molecular dipoles in their responses, although it facilitated students' discussion of electronegativity in determining the location of intermolecular forces which serves as the focus of this work.

The criteria behind selecting pairs of molecules were the following (1) single center molecules as examples on molecular polarity given to students in this population also used single center molecules, (2) the difference in electronegativity is equal to or higher than 0.5 because that is the cut off these students learn for the bond to be considered polar covalent, and (3) molecules of varying shapes to make sure not all molecules are linear. Some of the molecules selected are not readily observed in nature or completely soluble; however, participants were not asked to rate these features and instead were asked to engage in the process of identifying the location of dipole−dipole forces as this process was modeled for them within the general chemistry curriculum.

Data Analysis

Interviews were transcribed verbatim using the audio files. Screenshots of sketches were taken from the screen recordings and embedded in the interview transcripts and aided to contextualize the participants' descriptions. The transcripts were read line by line by two researchers followed by meetings to inductively generate codes for location, basis for location, and the way students used electronegativity, as well as other ways when electronegativity was not used. Codes were applied to a subset of transcripts independently by two researchers who met and reviewed discrepancies, leading to refinement of codes and reapplication in an iterative process until codes were interpreted consistently. Once the codes were finalized, as shown in the Supporting Information, the codes were independently applied to all the transcripts and consensus coding occurred where each disagreement was discussed to come to an agreement on the application of each code. Pseudonyms for each of the 18 participants will be used while describing the results: Aryn, Bridgette, Chavan, Danh, Ethan, Feng, Georgia, Hari, Ivy, Jake, Kavita, Lam, Mason, Nhu, Olive, Peter, Quinn, and Ria. Gender-neutral pronouns will be used as information on participants' preferred pronouns was not collected. It is of note that the codes were developed inductively to describe what the participants did when asked to find the location and not to label the resources activated. Codes were then used to develop themes that parsimoniously described distinct variations in determining the location of intermolecular forces.[35] The resource framework was used after coding and thematizing was complete to understand why participants enacted the way they did. As a result, the resource perspective served to provide researchers a perspective of explaining participants' ways of approaching this task.

Trustworthiness

Credibility, transferability, dependability, and confirmability are the four tenants of trustworthiness in qualitative work to regulate the reliability of the research.[36] The researchers working on this study were two chemistry graduate students, a chemistry faculty member, and an undergraduate student who successfully completed general chemistry. As a result, the research group was familiar with the chemistry instruction at the research setting supporting credibility to the research design and data interpretation. Iterative analyses of the interviews and consensus coding were carried to mitigate researcher bias and to present students' original ideas. A description of the setting, participants, and exams is described in the Methods section of Participants to promote transferability to the extent it is possible. The interview process, recruitment of students, and coding processes are detailed to support dependability. Finally, to support confirmability, student quotes and drawings are presented within the results to allow the reader to evaluate the inferences made.

■ RESULTS

Themes in participants' responses were characterized by the approaches enacted while predicting the location of dipole−dipole forces. Approach is operationalized as the basis of electing the location of dipole−dipole forces that came from the collection of resources that were activated and applied. The aim of presenting each approach by describing the resources is to show which resource was activated, thus putting a spotlight on the participant's use of various resources depending on the task. Of note, participants were informed that dipole−dipole force exists *between* the molecules in each set, and the electronegativity values were also given to them. These cues may have prompted the approaches described, and the study is not able to capture the effect of these cues as they were consistent across all participants. The approaches identified in this study are summarized in Table 1.

To identify the location of dipole−dipole forces between two distinct molecules, the instruction modeled a process that requires activating a collection of resources: (1) determine the molecular geometry, (2) identify atoms that share a chemical bond, (3) subtract electronegativity values only between bonded atoms, (4) determine whether the difference is above 0.5 such that the bond is polar covalent, (5) draw bond dipoles toward the more electronegative atom among each pair of bonded atoms that have a polar covalent bond, (6) sum the vectors of bond dipoles to determine the molecular dipoles or molecular polarity, (7) know dipole−dipole intermolecular forces only occur between molecules, (8) know dipole−dipole intermolecular forces result from an attraction between a positive molecular dipole and a negative molecular dipole, and (9) draw a dotted line to represent a dipole−dipole attraction.

1: Opposite Charges Attract

Ten out of the 18 participants Aryn, Chavan, Georgia, Hari, Ivy, Jake, Lam, Nhu, Peter, and Ria were explicit that dipole−dipole occurs between positive and negative ends of a dipole, with variations on whether this occurred between molecules or within molecules. Ivy talks about assigning partial charges as they selected the location of interaction as fluorine in IF and selenium in SeO_2 and connected those two atoms to show where dipole−dipole exists between IF and SeO_2.

Interviewer: *Can you explain to me one more time what you mean by the negative dipole and the positive dipole?*

Ivy: *In this case, since F would have the more negative partial charge in the iodine monofluoride and then Se would have the positive dipole on the selenium dioxide. It makes sense that they're connected.*

In the excerpt above, Ivy reasons that dipole−dipole forces result from opposite charge attraction and occur between molecules from atoms that have opposite partial charges. Participants Nhu and Peter show evidence of positive and negative dipoles using their sketches. Figure 2 shows Nhu's final sketch where they drew dipole arrows in red and connected chlorine in CH_3Cl and hydrogen in HBr. Among the 10 participants who followed this approach, variations existed in how molecular dipole was determined that are detailed in approaches 1A, 1B, and 1C.

Figure 2. Nhu showing partial charges and dipole arrows with CH_3Cl and HBr. In red, dipole moments between carbon and chlorine going toward chlorine and between hydrogen and bromine going toward bromine. In red, partial positive on carbon, partial negative on chlorine, partial positive on hydrogen, and partial negative on bromine. In red, connected chlorine with partial negative to hydrogen with partial positive with dotted lines. In green, showing the other locations of interaction.

1A: Opposite Charges Attract; EN Differences of Bonded Atoms

Four participants consistently compared the electronegativity magnitudes only between bonded atoms, matching the modeled use of electronegativity values. For example, when given the SCl_2 and NH_3 prompt, Ria said, *"bonds between S and chloride [in SCl_2], and N and hydrogen [in NH_3] are all polar bonds because the difference between electronegativity of S and Cl is 0.5. It's [a] polar bond and the difference of electronegativity of N and H is 0.9 so it's [a] polar bond."* Ria is seen here comparing electronegativity values only between bonded atoms and based on the difference identified the sulfur to chlorine bonds and nitrogen to hydrogen bonds as polar bonds. Four other participants also used this approach but were not consistent in its use.

1B: Opposite Charges Attract; EN Differences between Atoms in Different Molecules

One participant used partial charges as a basis for attraction but did not consistently subtract electronegativity values only between bonded atoms. When given SCl_2 and NH_3, Chavan compared electronegativity magnitude between bonded atoms: *"[within SCl_2] between sulfur and chloride, chloride is more electronegative. So that would be the negative end...for these [within NH_3], the more negative one is nitrogen."* However, when asked where the dipole−dipole force would occur Chavan said, *"I'm gonna say that it might be with the chlorine [from SCl_2] and the hydrogen [from NH_3]."* After this, the interviewer asked if there was another pair of atoms that could exhibit dipole−dipole forces, and Chavan compared electronegativity values between sulfur from SCl_2 and nitrogen from NH_3, that is, atoms on different molecules:

Interviewer: *Okay. So is there any other pair of atoms that can have dipole−dipole?*

Chavan: *I think the sulfur [in SCl_2] and the nitrogen [in NH_3] might be able to, just because the electronegativity difference is 0.5.*

Interviewer: *So, you are comparing which atoms?*

Chavan: *Sulfur [in SCl_2] and nitrogen [in NH_3].*

Chavan's initial conception of dipole−dipole force location was based on the attraction of opposite charges. However, within the context of prompting for other dipole−dipole attractions, Chavan compared electronegativity values between atoms that are on different molecules. This process maintained the resource that electronegativity differences of 0.5 were required, although here the difference was used to identify a dipole−dipole attraction rather than a bond dipole.

1C: Opposite Charges Attract; EN Differences between Unbonded Atoms within One Molecule

As above, this approach used partial charges as a basis for attraction but adopted another way to determine where partial charges would take place. Lam compared electronegativity between bonded atoms; however, Lam also compared electronegativity between unbonded atoms within the same molecule. In Figure 3, Lam places a partial negative on chlorine explaining, *"the chlorine [in CH_3Cl] does have a stronger electronegativity than the hydrogen atoms [in CH_3Cl]. So that tells me that the chlorine is found to be partially negative."* Since based on the way Lam drew CH_3Cl as seen in Figure 3, chlorine and hydrogen are not bonded, Lam's approach did not subtract electronegativity values only between bonded atoms. Lam

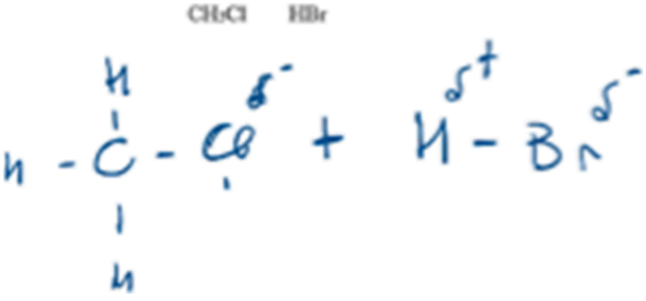


Figure 3. Lam showing partial charges on chlorine by comparing hydrogen and chlorine.

continues with HBr by comparing hydrogen's and bromine's electronegativity magnitudes and put partial charges saying, *"bromine has a stronger electronegativity so that tells me that it would also be partially negative, whereas the hydrogen would be partially positive."* In one instance, in CH_3Cl, Lam chose to compare electronegativity atoms between atoms of the same molecule that were not bonded, but in the other instance for the same prompt, in HBr, Lam compared electronegativity values between bonded atoms where unbonded atoms were not present. In this approach, Lam maintained a description that dipole−dipole forces occurred between molecules and resulted from an attraction of a positive molecular dipole and a negative molecular dipole.

2A: Differences in Electronegativity; Values Differ by More than 0.5

As opposed to approach 1 where partial charges are the basis for dipole−dipole forces, students in approach 2 cited differences in electronegativity as the basis. Aryn, Bridgette, Chavan, Ivy, and Olive identified whether the difference in electronegativity of atoms is above 0.5 to identify a dipole−dipole attraction rather than a bond dipole. Students with this approach varied in the location of dipole-dipole intermolecular forces, resulting in some intermolecular assignments and some intramolecular assignments.

Aryn compared electronegativity between bonded atoms and displayed dipole−dipole as within molecules. Aryn identified the location of dipole−dipole forces as between silicon and bromine within $SiHBr_3$ and between carbon and nitrogen within HCN and drew red circles on each bond to demonstrate it as shown in Figure 4. Aryn indicated the difference in electronegativities above 0.5 and below 1.7 as the rationale for this selection. Aryn only compared electronegativity values between bonded atoms within a molecule and used this comparison to assign dipole−dipole forces. Aryn further explained *"dipole−dipole force[s], I'm pretty sure, are not present in nonpolar bonds,"* as a justification for the "X" in Figure 4. Similarly, Bridgette described *"dipole−dipole includes polar bonds."* In essence, these responses identified atoms that share a chemical bond, subtracted electronegativity values only between bonded atoms, and determined whether the difference is above 0.5, and the bonds with electronegativity differences greater than 0.5 were assigned as the location of dipole−dipole forces. Thus, the activation of identifying electronegativity differences between bonded atoms greater than 0.5 was seen as an indication of the location of dipole−dipole forces and led to predicting the location of these forces within a molecule.

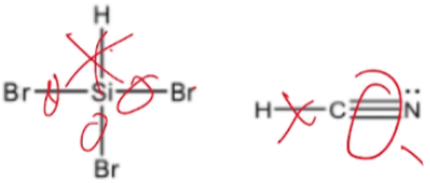


Figure 4. Aryn circling in red polar bonds and indicating with an "X" nonpolar bonds.

Chavan, Ivy, and Olive compared electronegativity values of atoms between the two molecules resulting in an *inter*molecular assignment of dipole−dipole forces. For example, when given, SCl_2 and NH_3, Olive compared electronegativity values between atoms on different molecules.

Olive: *For each of them, for the first one I've subtracted, the chlorine [in SCl_2] minus the hydrogen [in NH_3] so it is 3.0 [EN of chlorine] minus 2.1 [EN of hydrogen] which equals out to 0.9, which I believe is a polar attraction between them two. Then next I did nitrogen [in NH_3]...and chlorine [in SCl_2], which equals out to zero making it, I believe, nonpolar. I also did sulfur [SCl_2] and nitrogen [in NH_3], which gave me 0.4, which is nonpolar. Judging by how I got two nonpolars and only one that is polar and dipole−dipole is an attraction that is like polar, making the answer [location of dipole dipole] be chlorine and hydrogen.*

When the interviewer asked why electronegativity between bonded atoms was not compared, Olive said that the prompt was to find the dipole−dipole force between two molecules and not within. Within the context of this prompt, Olive activated the resource that dipole−dipole intermolecular forces only occur between molecules and that electronegativity values needed to be subtracted although not between bonded atoms. In essence, the cause-and-effect pattern of electronegativity values as the basis for dipole−dipole forces has been reversed in this approach. Instead, in this approach, participants activated the definition of intermolecular forces as between molecules to justify where comparisons of electronegativity values should occur.

While Aryn and Bridgette compared electronegativity values of atoms within the same molecule and located dipole−dipole as *intra*molecular; Chavan, Ivy, and Olive compared electronegativity values between atoms on different molecules and located dipole−dipole as *inter*molecular. Both groups of students were consistent in identifying whether the difference is above 0.5, and the atom pairs that met this threshold were identified as experiencing a dipole−dipole force of interaction. These two groups differed on whether dipole−dipole forces occurred between molecules, but neither group invoked partial charges or attributed dipole−dipole forces to partial charges.

2B: Differences in Electronegativity; Largest Difference in Values

Four participants, Ethan, Feng, Kavita, and Mason, identified the location of dipole−dipole forces as between atoms with the largest difference in electronegativity magnitudes, and because these happen to be between atoms on different molecules, participants in this approach located the dipole−dipole forces as *inter*molecular. For example, participant Ethan cited the largest difference in electronegativity as the lone reason for the location of dipole−dipole forces: *"I feel like the more [EN] difference there is between the two, the more that they're going to interact."* Following this approach, Ethan illustrated this interaction by drawing a dotted line between the bromine from $SiHBr_3$ and hydrogen from HCN (Figure 5), reasoning that they had the largest electronegativity difference of 2.8 among all the possible comparisons.

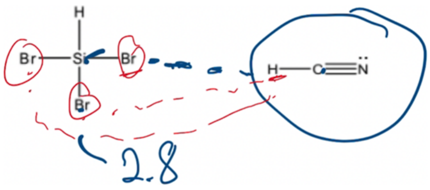


Figure 5. Ethan connecting bromine in $SiHBr_3$ and hydrogen in HCN by red dotted lines. The electronegativity difference of 2.8 (shown in blue) as the largest electronegativity difference.

This approach was not used consistently by Ethan, rather the prompt of $SiHBr_3$ and HCN was the only prompt in which they employed the approach of connecting atoms with the largest electronegativity difference. However, Feng and Kavita stayed consistent in their approach that the location of interaction are the atoms that have the largest differences in electronegativity for all four prompts. When Feng was asked to identify the location of interaction, they selected the chlorine from SCl_2 and hydrogen from NH_3 as shown in Figure 6 and reasoned *"they have the greatest difference in the electronegativity values."* These students subtracted electronegativity values but did not bring forth the model of subtracting values only between bonded atoms; however, Ethan did subtract values between bonded atoms to inform bond polarity on some of the prompts. These students were also cued to finding the largest difference in electronegativity values instead of comparing differences to 0.5, the threshold instruction set for labeling a bond polar covalent. Similar to approach 2A, in approach 2B, there was no explicit mention of partial charges or attributing dipole−dipole forces to partial charges. The assignment of dipole−dipole forces as *inter*molecular may be coincidental as the largest electronegativity differences in the prompts provided were between atoms on different molecules.

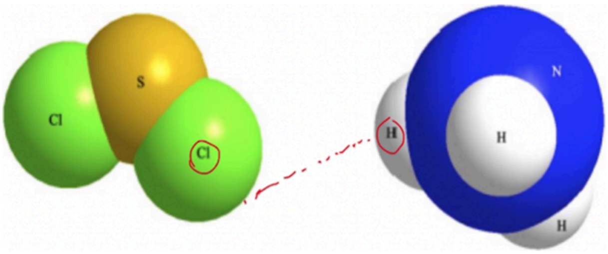


Figure 6. Feng connecting chlorine in SCl_2 and hydrogen in NH_3 by a red dotted line.

3: Size of Electronegativity Values

Three participants, Ethan, Lam, and Quinn, indicated that electronegativity values had to be used and focused on the size of the electronegativity values. They connected the atoms with the biggest magnitudes of electronegativity in each molecule to identify the location of the dipole−dipole force. For instance, Ethan connected chlorine from SCl_2 and nitrogen in NH_3 as the two between which dipole−dipole forces would occur as shown in Figure 7. When asked to provide the reasoning behind this choice, Ethan said *"it's [N in NH_3] more electronegative, so connect that to chlorine because that's [Cl in SCl_2] also the most electronegative."* In this approach, a resource was activated that the magnitude of electronegativity represents the reason behind the interaction between atoms, that is, the bigger the electronegativity, the greater the interaction. Another participant Lam reasoned why atoms attract by saying *"the N [in NH_3] also has the strongest EN and so that would make me think that N [in NH_3] and Cl [in SCl_2] would be attracted to each other."* Lam followed this approach as their reason for connection in two out of the four prompts. Quinn remained consistent in all four of the prompts and cited big EN values as the sole reason for dipole−dipole forces.

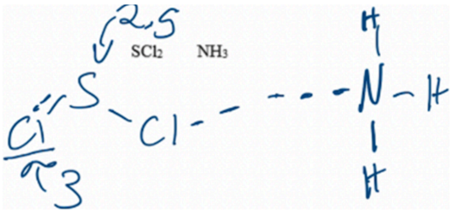


Figure 7. Ethan connecting chlorine in SCl_2 and nitrogen in NH_3 by blue dotted lines. The 2.5 is the electronegativity magnitude of sulfur and 3 is the electronegativity of chlorine.

Approach 3 also matches Talanquer's[37] description of "one-reason decision making". This heuristic is described as a series of steps learners may use to reduce the complexity of problems. In this heuristic, the learner searches for a cue or explicit feature to differentiate options, compares values of the selected cue for each alternative, and stops the search when a cue is found that can be used to make a choice. In approach 3, the cue is the electronegativity values and the comparison results in identifying the largest electronegativity value, which becomes a rationalization for the location of dipole−dipole forces. This approach differs from approaches 1 (opposite charges attract) and 2 (electronegativity differences) as approach 3 describes a resource on the meaning of electronegativity unique from the other approaches. Similar to approach 2B, the assignment of dipole−dipole forces as *inter*molecular in approach 3 may be coincidental as the largest electronegativity values in each prompt provided were from atoms on different molecules.

4: Atomic Size

Atomic size was utilized by one participant. Ethan cited atomic size as the reason why atoms will experience attraction. In the excerpt below, Ethan is given IF and SeO_2 and asked where the dipole−dipole occurs between the two molecules.

Ethan: *The initial thought as I'm looking at the picture [molecules of IF and SeO_2] is that, in this first one [molecule] over here [on the left], the I [in IF] is significantly bigger than the F [in IF]...It makes me feel that the I should have more attraction to it [molecule on the right].*

Interviewer: *If any interaction were to occur between this molecule on the left [IF] and another molecule [SeO_2], then it would be attached to the I?*

Ethan: *Yes. like the I [in IF] would attract Se [in SeO_2]...with them [atoms] being bigger makes me feel like I want to connect these two [I in IF and Se in SeO_2].*

Ethan cites iodine in IF because it has the largest atomic size and selenium has the largest atomic size in SeO_2 and concludes these two atoms will be the location of attraction between the two molecules. It is believed that the focus on atomic size may have resulted from the context of the given representation of the molecules. Ethan adopted this approach only for the prompts that use the ball-and-stick or space-filling models (see Figure 1, version 1, prompts 3 and 4) which were the only representations that provide atomic size as an explicit feature. This explanation would concur with Ethan's reliance on electronegativity values with the first two prompts when atomic size was not explicit in the representations. Within the context of representations where atomic size was explicit, Ethan activated the resource that dipole−dipole occurs between molecules and activated a resource where atomic size predicted the location of dipole−dipole forces, while no longer activating resources pertaining to electronegativity values, bond dipoles, molecular polarity, or the attraction of opposite charges.

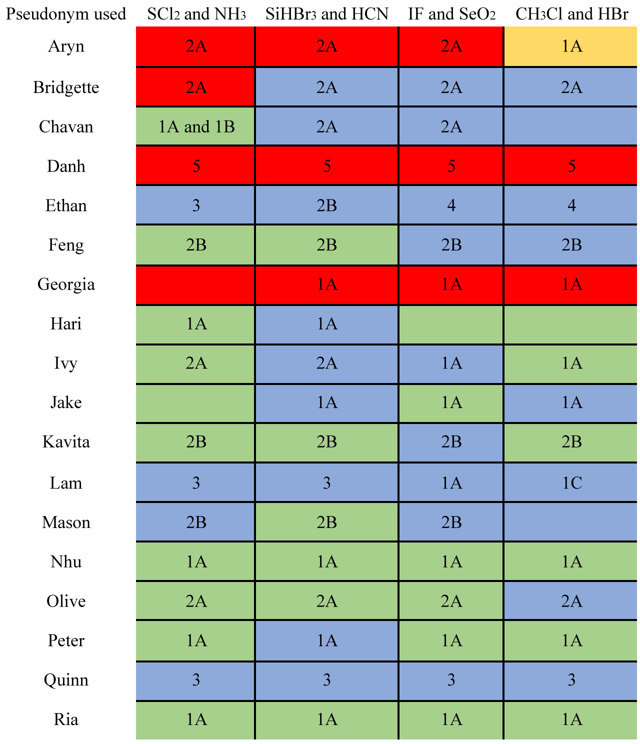
5: Molecular Shape

Danh followed an approach distinct from the other approaches by citing only molecular shape when determining the location of the dipole−dipole forces and was consistent across the four prompts. When given SCl_2 and NH_3, they stated *"because dipole−dipole exists where...molecules are bent, and these [sulfur to chlorine bonds] are in a bent shape right here. So these two bonds would be dipole−dipole."* When asked to explain why dipole−dipole occurs between molecules that are bent, Danh said, *"because the bonds are stronger on these ends [sulfur to chlorine bonds in* SCl_2*]. Since they're stronger, they pull more together, as opposed to, a linear structure. They're [bonds] usually stronger because I know for water, the hydrogens [are] polar. And because they're polar, they can, like, attract other molecules easier. And because they have a higher electronegativity."* Of note, in Danh's lexicon, atoms are assigned the characteristic of being polar, and the bonds inside a molecule are assigned a dipole−dipole force. Danh's reasoning appears based on familiarity with a water molecule having a bent shape and polar characteristics, which is then mapped on to other molecules with a bent shape. Consistent to this reasoning, when asked whether there was a dipole in IF, Danh replied there was not a dipole because it did not show a bent geometry. When asked how they used electronegativity (EN) values given to them, they said *"I barely even acknowledge the EN values. I think just by looking at this one [set], I could tell which one [molecule] has stronger IMFs [intermolecular forces]. And that would be the* SeO_2*"*, reaffirming Danh's contention that dipole−dipole forces are within a molecule. Danh activates the resource of molecular geometry and that asymmetric molecules commonly show molecular polarity and engage in dipole−dipole interactions. Thus, in the collection of resources, Danh activates resources about molecular geometry but activating resources pertaining to electronegativity, bond or molecular polarity, and partial charges were not observed.

Considerations across Participants

To examine consistency in approaches among participants, the approaches for each participant are presented in Figure 8. This figure also includes a color background to indicate the accuracy of the predicted location and whether the predicted location was *inter*molecular or *intra*molecular. Green and blue backgrounds indicated the dipole−dipole was located as *inter*molecular, with green indicating a correct location and blue an incorrect location. Of the 18 interview participants, 14 consistently showed dipole−dipole as an *inter*molecular force. This figure also indicates the approach used by each participant at each prompt. Participants in this study were notably consistent in the approaches they adopted. Only five participants, Aryn, Chavan, Ethan, Ivy, and Lam, changed their approach across the prompts.

Despite the general consistency in students' approaches, only five students, Hari, Jake, Nhu, Peter, and Ria, consistently used approach 1A, with electronegativity comparisons of bonded atoms to determine polarity and then opposite charges attract as the location of the dipole−dipole force. Of those, only Nhu and Ria used this approach and identified the correct location for each molecule pair. It is also worth noting instances where participants used an approach wherein the resource of assigning partial charges was not seen and yet were able to identify the location correctly. For instance, Feng, Kavita, Mason, and Olive consistently used approaches 2A or 2B (using electronegativity differences as the location of intermolecular forces), and each indicated the correct location at least once, with Kavita and Olive doing so on three of the four molecule pairs. Approaches 3, 4, or 5, relying on size of electronegativity values, atomic size, and molecular shape, respectively, did not result in the correct location for the dipole−dipole force.



Pseudonym used	SCl_2 and NH_3	$SiHBr_3$ and HCN	IF and SeO_2	CH_3Cl and HBr
Aryn	🟥 2A	🟥 2A	🟥 2A	🟨 1A
Bridgette	🟥 2A	🟦 2A	🟦 2A	🟦 2A
Chavan	🟩 1A and 1B	🟦 2A	🟦 2A	🟦
Danh	🟥 5	🟥 5	🟥 5	🟥 5
Ethan	🟦 3	🟦 2B	🟦 4	🟦 4
Feng	🟩 2B	🟩 2B	🟦 2B	🟦 2B
Georgia	🟥	🟥 1A	🟥 1A	🟥 1A
Hari	🟩 1A	🟦 1A	🟩	🟩
Ivy	🟩 2A	🟩 2A	🟦 1A	🟩 1A
Jake	🟩	🟦 1A	🟩 1A	🟦 1A
Kavita	🟩 2B	🟩 2B	🟦 2B	🟩 2B
Lam	🟦 3	🟦 3	🟦 1A	🟦 1C
Mason	🟦 2B	🟩 2B	🟦 2B	🟦
Nhu	🟩 1A	🟩 1A	🟩 1A	🟩 1A
Olive	🟩 2A	🟩 2A	🟩 2A	🟦 2A
Peter	🟩 1A	🟦 1A	🟩 1A	🟩 1A
Quinn	🟦 3	🟦 3	🟦 3	🟦 3
Ria	🟩 1A	🟩 1A	🟩 1A	🟩 1A

Figure 8. Red refers to intramolecular. Green is intermolecular correct. Blue is intermolecular incorrect. Yellow is intra- and intermolecular. Text in the cells are approaches based on Table 1. No text in cell: approach unable to be identified.

■ DISCUSSION

A slight majority of the participants demonstrated the resource of opposite charges attraction as a basis for dipole−dipole forces (approach 1). Even so, some of these participants activated the resource of comparing electronegativity values but not within the context of comparing atoms that share a chemical bond and instead compared atoms that were not bonded or between atoms from different molecules (approaches 1B and 1C). The comparison of electronegativity values outside of bonded atoms was also manifested in approaches 2A and 2B where it occurred without the resource of partial charges. In these instances, differences in electronegativity became the identifier of dipole−dipole interactions rather than the identifier of a polar covalent bond. This application of electronegativity matches a prior report in the research literature where undergraduate students compared electronegativity values between atoms located in different molecules.[38]

In approach 3, participants activated a resource that defined electronegativity in a unique way, where the largest magnitude in electronegativity was responsible for attraction. This may represent assigning innate characteristics to atoms that cause a particular atom to attract other atoms on different molecules. This has been described by Talanquer as atomic compositionism[5] and matches a call to promote the emergent properties of molecules.[39] Molecular polarity is an emergent property of chemical bonds and molecular shape, and intermolecular forces are an emergent property of a system composed of multiple molecules. Instead, approach 3 supplants these emergent properties with an innate characteristic whereby atoms can be the cause of dipole−dipole forces via the magnitude of their electronegativity values. Alternatively, approach 3 may also be enacted as a function of the cues given in the prompt as students see the electronegativity values and presume they must be used. This explanation matches the experience of Ethan, who switched from approach 3 to approach 4 when the prompt made atomic size an explicit feature. Further investigation on the cuing effect of the prompt is needed to better understand the interplay between the cuing features of the prompt and students' internal conceptions.

■ TEACHING IMPLICATIONS

Furthering an understanding of students' approaches on dipole−dipole forces provides insight into students' rationalization efforts with this topic. Instructors can then utilize this understanding to engage students in further exploration.[40] These findings suggest that instruction and assessment on the topic of intermolecular forces may benefit from a more explicit integration of how electronegativity is used when introducing and discussing intermolecular forces. Typically, electronegativity is introduced accompanying molecular shape and used as the determination of molecular polarity; from there, it may be presumed that students' proficiencies with this skill will carry over when intermolecular forces are introduced. This study found that this presumption would not be supported. Most students were proficient in recognizing the need for comparing electronegativity values but varied in identifying atoms that can be compared or in the utilization of this comparison to determine the location of dipole−dipole intermolecular forces (as demonstrated in approaches 1B, 2A, 2B, and 3). This alternative use of electronegativity may not be apparent to instructors when current instruction introduces electronegativity only within single molecules under the topic of molecular polarity. In short, the current general chemistry curriculum design, which focuses on electronegativity primarily with single molecule systems, is unlikely to support students delineating where to make electronegativity comparisons when multiple molecule systems are present. Instruction may benefit by presenting and assessing the appropriate use of electronegativity values in systems of more than one molecule including systems where the two molecules are distinct. Using systems with more than one molecule would allow instruction to highlight electronegativity as intended only for comparisons between bonded atoms.

This work also highlights the potential benefits of developing instructional techniques and assessment that engage in the process of identifying the location of intermolecular forces. Assessments which only require a prediction of location are not sufficient for eliciting these processes. Kavita and Olive were able to identify the correct location on three of the four molecular pairs while using differences in electronegativity as a proxy for location. Students using differences in electronegativity as a proxy for the location of dipole−dipole forces may have this process reinforced when they receive assessments that ask only about the location. Instead, students would benefit from describing the process for determining the location and receiving feedback on their stated processes.

■ RESEARCH IMPLICATIONS

The approaches detailed herein may support designing an instrument that is sensitive to the variations in approach; such an instrument could support a large-scale investigation into the prevalence of these approaches. Past work developed a concept inventory to determine student understanding of intermolecular forces with a focus on determining the type of intermolecular forces (e.g., hydrogen bonding) and the relationship of physical properties (e.g., boiling point, vapor pressure) to the strength of intermolecular forces.[9] While there is a need for measuring student proficiencies with these tasks, the work presented herein calls attention to the additional task of utilizing electronegativity values to determine the location of intermolecular forces. This study also calls attention to the possibility of students making correct predictions on the location of dipole−dipole forces, while engaging in an incorrect process.[11] Therefore, the proposed inventory could be synthesized utilizing questions similar to the ones presented to students in this study. Instrument design would benefit by including tiered questions, or separate items, that prompt students to predict the location of the intermolecular force and select the process in determining the location. The approaches listed herein could serve as plausible distractors for the latter. These questions would assess students' use of electronegativity to identify bond dipoles and use of molecular dipoles to ascertain the existence of dipole−dipole interactions between two different molecules. The information gained from such an instrument could guide instructional design and formative and summative assessment.

Another potentially fruitful research perspective would be to investigate the impact of curriculum changes that adopted the integration of electronegativity into systems of multiple molecules when presenting intermolecular forces in general chemistry. It is reasonable to hypothesize that such an integration would strengthen students' understanding of molecular polarity, particularly when given systems that comprise multiple molecules. Since organic chemistry strongly relies on modeling molecular polarity in multiple molecule systems (e.g., reaction mechanisms), this hypothesis would predict that enacting the proposed curriculum changes in general chemistry may improve students' understanding within organic chemistry. Future research could investigate this possibility.

The current study also found the majority of student responses were consistent across the four prompts, suggesting these approaches may remain consistent across varying contexts.[41] Future research studying student approaches across a wider variety of contexts could prove fruitful. Other contexts may include investigating students' processes without electronegativity values provided or with a scaffolded prompt to identify molecular dipoles. By examining students' resource use as context changes, it can inform instruction on contextual cues that can support student success.

■ LIMITATIONS

This study should be framed within hermeneutic considerations; that is, if another researcher were to look at these data, they may have engaged in a different analytic perspective and reached alternative conclusions. This work is qualitative in nature; it does not make direct claims of generalizability but provides descriptions of the variety of ways students experience the phenomenon. Further, this study collected data from a single institution, where the curriculum in place contributed to the students' approaches. Collecting data from multiple institutions, or a broader sample, may identify further variety of ways that students experience the phenomenon.

This study did not investigate the impact of cueing that may have arisen from the interview directions to identify the pair(s) of atoms where the strongest intermolecular force occurred or from providing electronegativity values. Providing the electronegativity values is in line with assessments typically given at the research setting, but other research settings that rely on a qualitative determination of relative electronegativity may manifest different student approaches. It is of note that, even with the explicit use of the word *between*, many participants located the dipole−dipole force *intra*molecularly.

It is also worth noting that the interview prompt asked participants to identify the pair(s) of atoms where the strongest intermolecular force would occur, while some of the molecules' dipoles are in an interatomic region. It is unknown whether students would engage in the approaches described herein if they were directed to draw intermolecular forces with a less directive statement (e.g., draw the location of the dipole−dipole force).

Finally, the results of this study may be impacted by the variations in molecular representations used. For example, it is unclear if approach 4, the use of atomic size, was a result of relative atomic size being explicit in the representation. Settings that rely on singular representation types may not manifest the same set of student approaches as found here.

CONCLUSIONS

The concept of intermolecular forces offers a high degree of explanative utility in relating submicroscopic entities to macroscopic properties and in understanding multimolecular systems, making it a foundational topic in a chemistry curriculum. This study found general chemistry students were often familiar with comparing electronegativity values but differed in where the comparisons should take place (e.g., between atoms from differing molecules) and how this comparison can lead to the identification of the location of dipole−dipole forces. The current general chemistry curriculum design, which focuses on electronegativity primarily with single molecule systems, is unlikely to support students delineating where to make electronegativity comparisons when multiple molecule systems are present. The context of multiple molecule systems is essential for understanding molecular interactions which become a focus in organic chemistry and biochemistry. An instructional implication arising from this work is the potential benefit of integrating electronegativity and the determination of molecular polarity in systems composed of multiple molecules into the introduction and assessment of intermolecular forces.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.2c01230.

> Interview protocol; Codebook for how students predicted the location of intermolecular forces; Selection of location of interaction by participants (PDF; DOCX)

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Notes

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