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# To See IMFs on a Surface of Glass: Causal Mechanistic Reasoning and Intermolecular Forces in the Undergraduate Chemistry Lab

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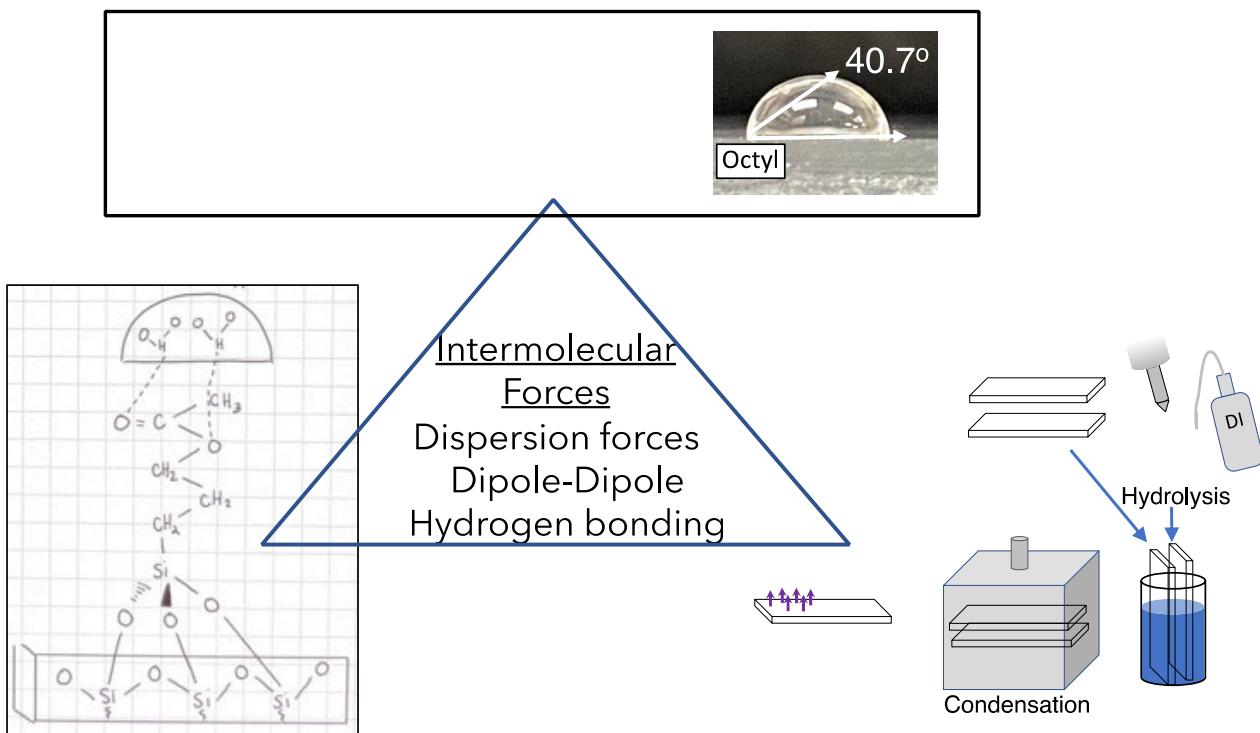
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## ABSTRACT

Intermolecular forces (IMF) are a fundamental concept of chemistry and one that is integral to students' understanding of the properties and interactions of matter. Despite this, students struggle to apply IMFs to real phenomena in their world. Here we describe a first-semester general chemistry laboratory in which students 10 functionalize the surface of glass slides and observe the interaction of water and heptane drops with the surface, allowing them to integrate IMF, molecular modeling, and causal mechanistic reasoning to explain observable and measurable phenomena. In the activity, students perform and describe a series of simple reactions that covalently bond the silane molecules acetoxypropyltrimethoxysilane and octyltrimethoxysilane to the glass surface. They then characterize the slides by adding drops of water to the modified slide, taking profile pictures with their cell 15 phones, and determining the drop half angles from the pictures using *ImageJ* software. Students also add drops of heptane to the slides and observe their interactions with the slides, contrasting those with the interactions of the water drops. This lab activity invites students to consider the material of the lab on the macroscopic and submicroscopic levels as they describe the functionalization of glass slides, observe the interaction of the modified 20 and unmodified slides with drops of water and heptane, and then construct explanations that use and reinforce their learning of IMFs and molecular structures. The experimental procedure and data collection proved to be robust, with most students producing data that was consistent with expectations and that supported their claims about the IMFs between water molecules and between the water molecules and the surface.

## GRAPHICAL ABSTRACT

# IMFs on a Surface of Glass



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## KEYWORDS

First-year undergraduate/General Laboratory Instruction, Analytical Chemistry, Causal Mechanistic

30 Reasoning, Intermolecular Forces, Contact Angle, Silane, glass, Cell Phone, Hands-On Learning/Manipulatives, Material Science, Surface Science

## INTRODUCTION

There has been a strong emphasis to move chemistry education from its historically observational

and descriptive nature to an explanatory process in which building mechanistic explanations are seen

35 as the path to greater understanding of the natural world and well-organized chemical knowledge.<sup>1</sup>

One area of interest has been how students explain various chemical phenomena through causal

mechanistic reasoning (CMR). In CMR, students consider a phenomenon such as boiling point,

solubility, or a chemical reaction and explain it using concepts of chemistry where the explanation

involves (a) structural components at scalar levels below the phenomenon (e.g., particles, molecules,

40 atoms, ions, or electrons), (b) properties and/or behaviors of these components (e.g., charge or vibration), and (c) connecting these properties and behavior back to the phenomenon.<sup>2,3</sup> In this form of reasoning, students engage in the crosscutting concept of cause and effect and use science and engineering practices such as modeling.<sup>4,5</sup> With the recent focus on CMR as a framework of chemistry education,<sup>1,2,6-9</sup> researchers and practitioners have proposed a number of areas in chemistry where 45 this is appropriate. One of these is intermolecular forces.

50 Intermolecular forces (IMFs) are the interactions that occur between molecules or between molecules and ions. These forces, which include hydrogen bonding, dipole-dipole interactions, ion-dipole interactions, and London dispersion forces, arise from the attraction between partial charges or temporary dipoles on adjacent molecules and play a crucial role in determining the behavior of 55 substances in various states of matter.<sup>10</sup> While IMFs are critical to chemistry education, they have proven to be a difficult concept for many students.<sup>11-14</sup> A significant amount of research has been done into students understanding of IMFs as a discrete concept unrelated to a phenomenon.<sup>11,14-17</sup> Work has also been done in how instructors teach IMFs<sup>18</sup> and activities to improve students understanding of IMFs.<sup>19-24</sup> Other research has looked at how students use IMFs to explain and predict phenomena, 60 These include analysis of how students explained: melting point and boiling point data,<sup>25-28</sup> solubility,<sup>29</sup> heats of vaporization,<sup>30</sup> thin layer chromatography,<sup>31-34</sup> gas chromatography,<sup>33,35-37</sup> and chemical and physical properties of organic acids.<sup>38</sup> The importance of IMFs in chemistry education is nowhere more prominently displayed than in the development of an inquiry-based lab course 65 structured around IMFs by Harmon *et al.*<sup>13</sup> Through backward design, they considered the knowledge and skills necessary for lab work and then looked at how the understanding of IMFs intersected with those concept and skills culminating in a caffeine extraction practical from which they developed the course curriculum. Clearly IMFs are well suited to CMR because of their inherent molecular and electronic scale and the modeling involved in understanding them.

70 This paper describes a novel general chemistry laboratory activity in which students produce 65 functionalized glass slides, observe the interaction of liquids with their surfaces, and then explain the interaction using molecular structure and IMFs. We also provide information on how the experience impacts learning.

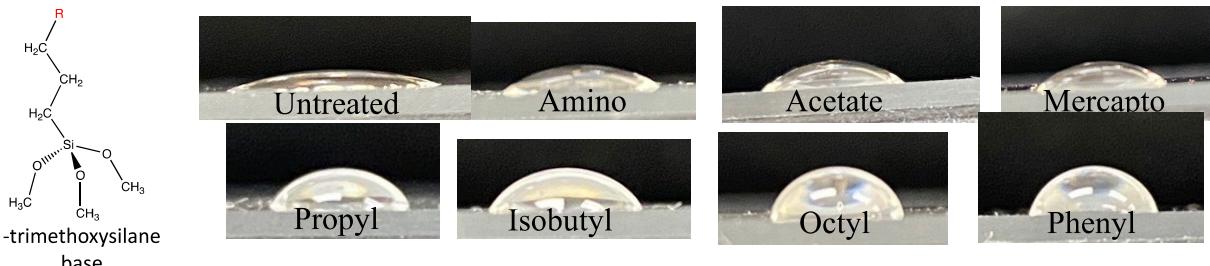
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## EXPERIMENTAL OVERVIEW

In the summer of 2022, we recognized the need to include an experiment explicitly covering IMFs in a new general chemistry sequence. The learning outcomes were that students would observe and/or measure a chemical phenomenon and explain their data and the phenomenon using causal mechanistic reasoning with molecular structures and IMFs. Initially we used a vapor pressure lab developed by Fitzgerald *et al.* in which students determine vapor pressures of organic compounds and heats of vaporization, which they relate to the IMFs in the compounds.<sup>30</sup> While this is a creative and well-structured lab, when we analyzed students' data and interpretations as well as TAs' feedback, it was apparent that the dexterity and precision necessary to set up the experiment and the long chain of calculations and inferences, was negatively impacting students' learning. In the following summer, we explored other materials and phenomena that have been reported as possible applications of the concepts of IMFs to observable chemical phenomena. These included melting point measurements,<sup>39</sup> solubility of alcohols,<sup>29</sup> and TLC of both organic molecules<sup>31,34</sup> and disperse dyes. These had varying degrees of promise in engaging students in the three domains of learning—cognitive, psychomotor, and affective—and as vehicles to explore the crosscutting concepts of cause and effect and structure and function. As this would be the final laboratory of the course, we also wanted to incorporate chemical change in the activity. We found a possible candidate in a previously developed biosensor activity involving glass slides, functionalized silanes, and a drop of water.

The original experiment for our work was developed within a biosensor CURE module for the Center for Authentic Science Practice in Education (CASPiE)<sup>40,41</sup> by Albena Ivanisevic (unpublished material). In it, the surface of a common glass microscope slide is modified using trialkoxysilanes, characterized using contact angle goniometry, and labeled with fluorescent tags. This module was subsequently used in a pre-college summer program in 2013-2014 by students in our university's Latino Health Science Enrichment Program (LAHSEP) to provide participants with opportunities to accomplish undergraduate research. The students experimented with various changes to the procedure, carrying out authentic experimentation by developing protocols for modifying and characterizing the surfaces of glass slide. We expanded on that work by having students use different alkoxy silanes with a focus on functional groups that would provide for variations in the interaction of

the glass surface with water droplets (Figure 1). As our objectives were for students to both engage in chemical change and to analyze data in the context of IMFs, we dropped the fluorescent tagging and instead focused on modification and characterization of the glass surface itself.



100 Figure 1. (left) Schematic diagram of -trimethoxysilane base used in developing the experiment. (right) Examples of water drop profiles from the early stages of testing alkoxy silanes. Names represent the R group which extended above the surface after the covalent bonding of the trimethoxysilanes onto the slide surface. Untreated is type II soda-lime glass slide out of the box and the Propyl is the alkoxy silane without a functional group.

105 Silanes are an important class of compounds because of their ability to self-assemble and form monolayers on glass surfaces. We are using the term silane as a general category name for those compounds containing a central silicon surrounded by organic groups, at least one of which is an alkoxy (Figure 2).<sup>42</sup> The use of alkoxy silanes on silica surfaces to form monolayers has been extensively studied,<sup>43–51</sup> and is important in a wide range of applications including electronics, biomedical, and material sciences, making it relevant as an object of study in chemistry education.<sup>52,53</sup>

110 For the development of this laboratory we used trimethoxysilanes because of their availability, their widespread use in surface science chemistry, and the simplicity and robustness of their reactivity (i.e., hydrolysis in water, hydrogen bonding to hydroxyls on glass, and condensation with moderate heat).<sup>54</sup>

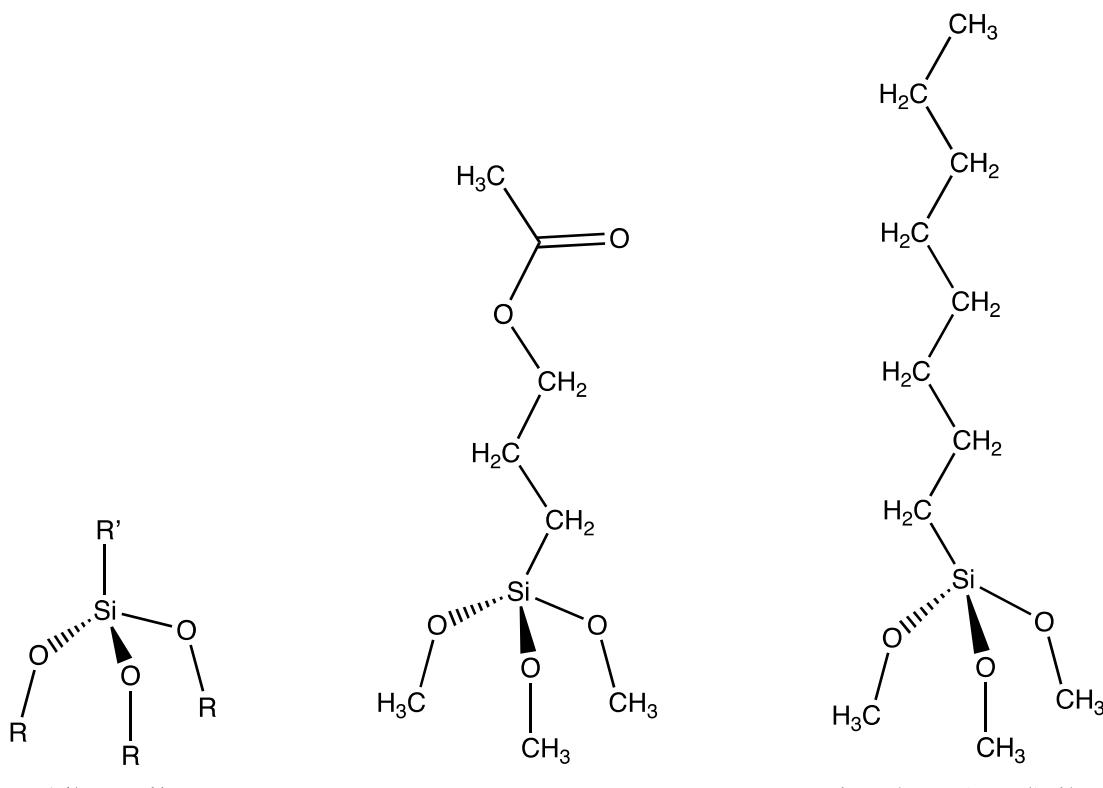


Figure 2. Scheme showing: (left) the general structure of silanes where R is an alkyl and R' is an organic group and (middle and right) the silanes used in this laboratory. Silanes by definition will have one, two or three alkoxy's attached to the silicon.

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### LEARNING OBJECTIVES

As a culminating experiment to the first-semester course, the objectives for this lab extended

beyond understanding IMFs to also include chemical reactions. Students were:

- to explain the chemical reactions that were occurring during the steps of the surface modification;
- to model, on the submicroscopic level, the processes occurring during surface modification; and
- to use CMR to explain the observable and measurable phenomena of liquid-surface interaction to molecular structures and IMFs.

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As the laboratory course is structured within the framework of three-dimensional learning, the

outcomes were developed in conjunction with the discipline core ideas (DCIs) from the anchoring concepts content maps for general chemistry (ACCM),<sup>55</sup> the science and engineering practices (SEPs) and the crosscutting concepts (CCCs) which are both from Next Generation Science Standards (NGSS).<sup>56</sup> The specific list of these can be found in the Supporting Information.

## THE EXPERIMENT

This activity was designed for a general chemistry laboratory class at a large midwestern urban university serving a population with no majority ethnic or racial demographic. The university is a Minority-Serving Institute (MSI), an Asian American and Native American Pacific Islander-Serving Institution (AANAPISI), and Hispanic-Serving Institute (HIS). The laboratory is a two-credit, one-semester course taught independently of the introductory lecture course, though most students are enrolled in both lecture and lab. It includes 12 labs over a 15-week semester and serves students in traditional chemistry and biochemistry tracks, as well as other STEM majors, and preprofessional tracks—including nursing, pre-pharmacy, and pre-medicine. Lab periods are three hours long, contain up to 24 students, and are led by one graduate teaching assistant (TA). This experiment is intended as the final lab of the first-semester and can be easily completed in under three hours, including multiple “Pause and Reflect” events that are a general pedagogical tool in the course.

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### Experiment Structure

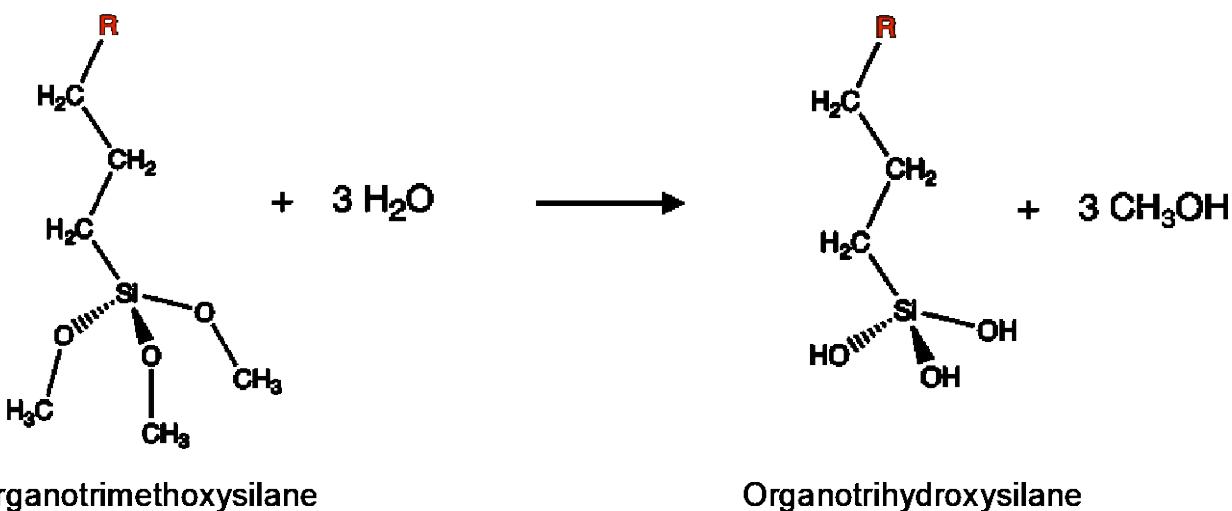
The activity has three parts (Table 1). The first part involves chemical reactions to produce the modified glass slides (Figure 3); the second part is the characterization of the surface of the slide (Figure 4); and the third part is the construction of causal mechanistic explanations of the observation of the liquid on the slide. Interspersed through these sections were reflective exercises as summarized in Table 1. Students also received an asynchronous lecture about the concepts for the lab. The slides from the lecture are provided in the Supporting Information.

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**Table 1. Steps in the laboratory procedure documenting the relationship between the “pause and reflect” events and the procedures in the experiment.**

Experiment Steps	Procedure Steps	Pause and Reflect Steps
<b>Part 1: Producing the Modified Slides</b>		
	Collaborate and choose silane	Draw the chosen silane
<b>Hydrolysis</b>	Mix the silane and water	Draw product of hydrolysis
<b>Hydrogen bonding</b>	Add slides to the solution	Draw and label the hydrogen bonds between the silanol and the glass surface
<b>Condensation</b>	Heat the slides in the oven	Draw the surface of the functionalized slide
<b>Part 2: Data Collection</b>		
<b>Water drop on the pipet</b>	Photograph a drop of water on the pipet	
<b>Water drop on a slide</b>	Photograph the profile of water drop on the slide	<ul style="list-style-type: none"> <li>Describe the difference between drop on the pipet and on the slide</li> <li>Explain the difference between the drop on the pipet and on the slide</li> </ul>
<b>Water drops on functionalized slides</b>	Photograph the profiles of water drops on the functionalized slides	
<b>Heptane drops on slides</b>	Photograph a drop of heptane on the slides	
<b>Part 3: Data Analysis</b>		
	Determine the half angle of water drops on each slide using <i>ImageJ</i> software	Post Lab questions in the lab report <ul style="list-style-type: none"> <li>Draw a molecular diagram of the surface of the slide and a water drop</li> <li>Draw the IMFs present</li> <li>Explain the differences in drop half angles between the three glass slides</li> <li>Explain why the heptane interacts differently than the water to the glass slides.</li> </ul>

(a)



(b)

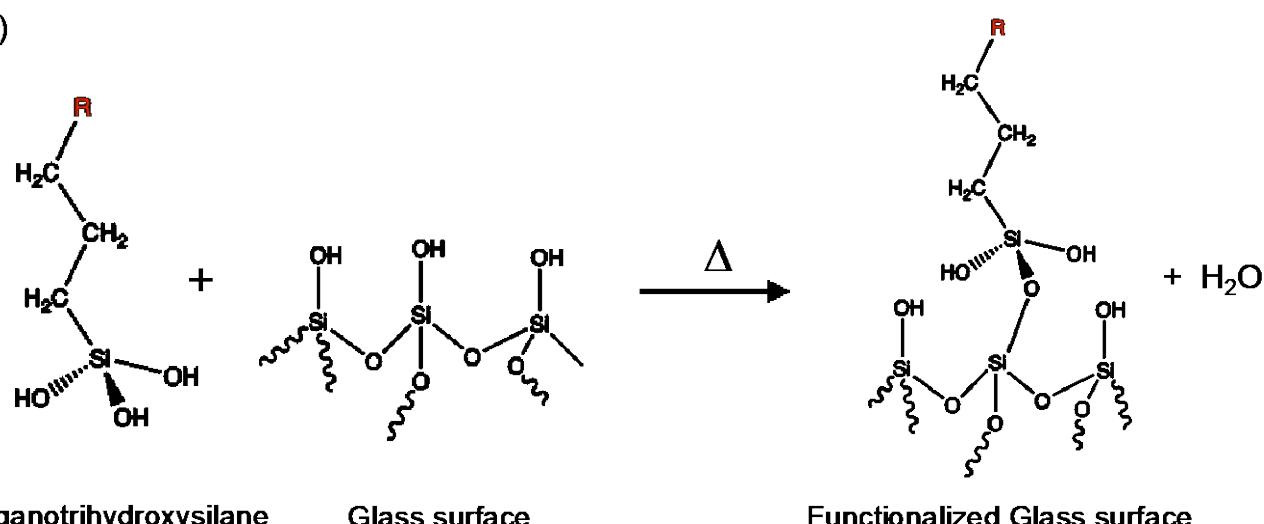
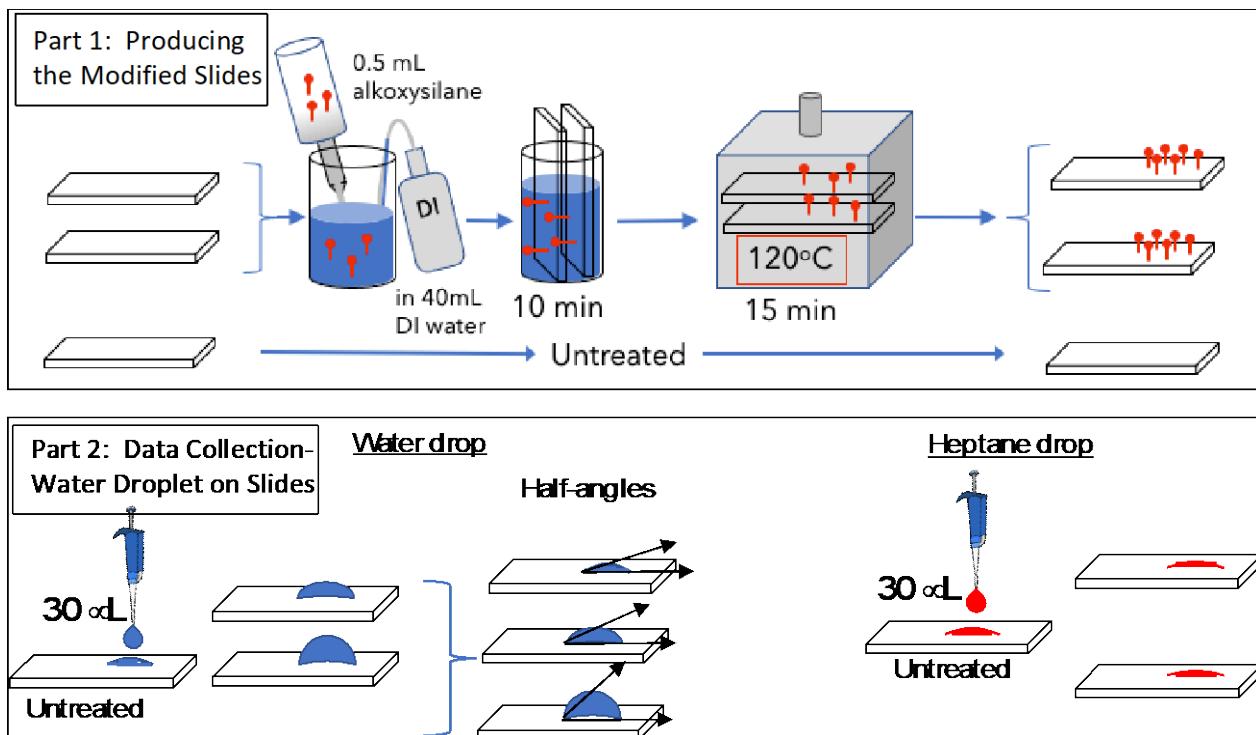


Figure 3. (a) Hydrolysis of organotrimethoxysilane. (b) Condensation of organotrihydroxysilane with the surface.

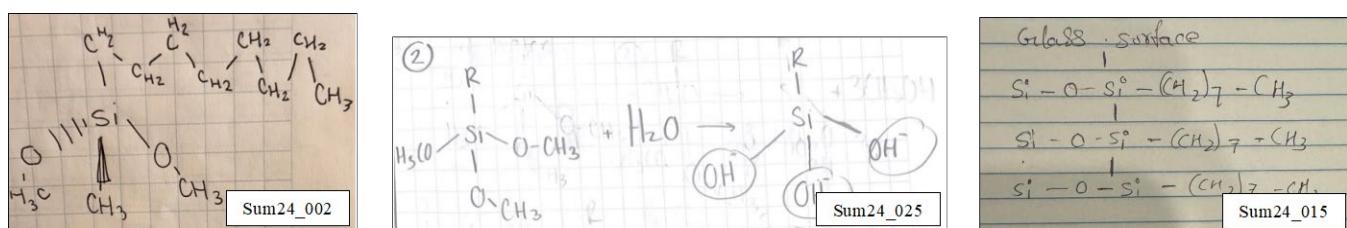


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Figure 4. Schematic diagram of (top) the functionalizing of the glass slides and (bottom) the characterization of the surface of the glass slide.

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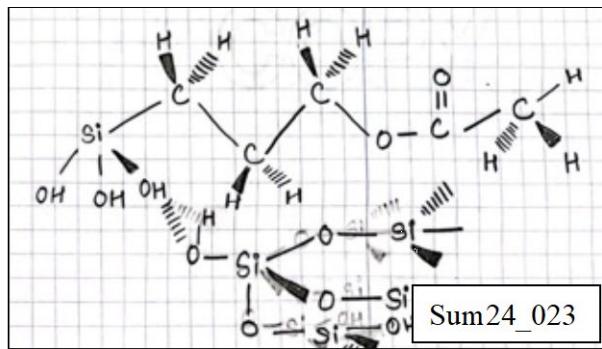
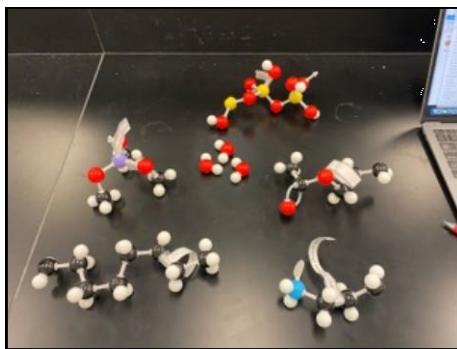
The procedure to modify the slides is straightforward and, while not exceedingly exciting (e.g., there were no color or state changes and no significant energy transfers), it lent itself well to students' thinking on a submicroscopic level. The lab was scaffolded to direct students to think about aspects of the laboratory they might not typically consider in their haste to finish as quickly as possible.<sup>57</sup> As students functionalized their slides with silanes, they were required to stop, reflect, and write on a submicroscopic level about what they had done or seen by drawing or describing molecules at that stage in the reaction (e.g., drawing the silanol after the trimethoxysilane reacted with water)(figure 5).



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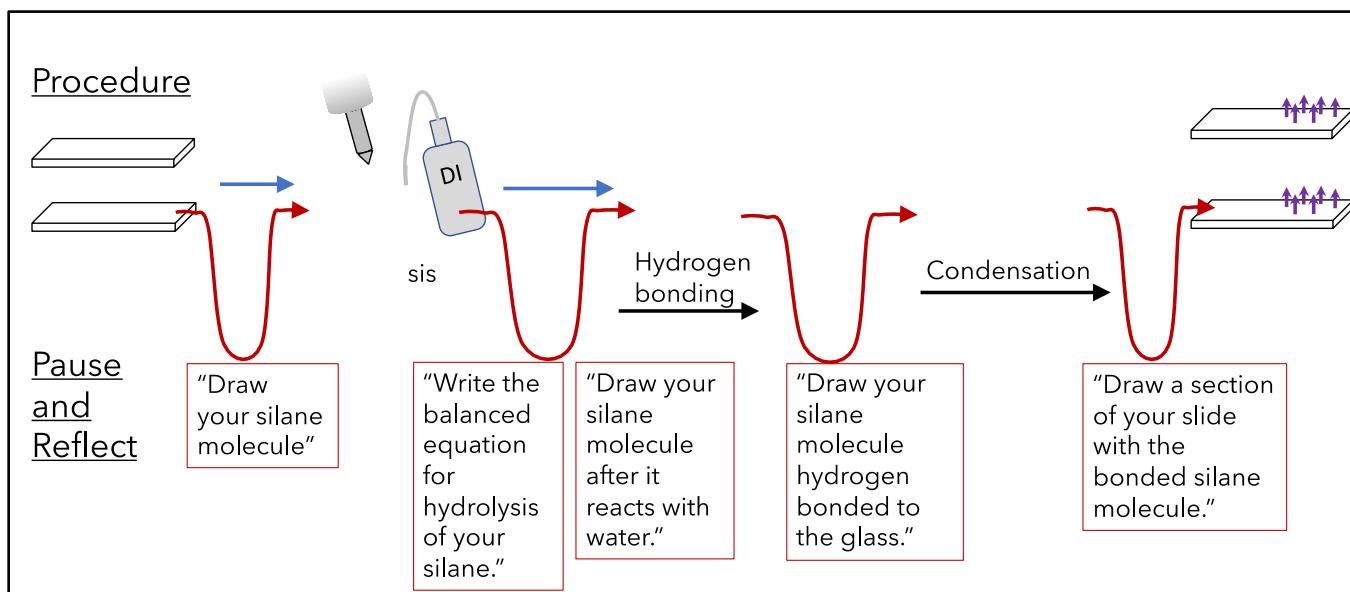
Figure 5. Examples of student drawing in response to lab prompts: (left) In your lab notebook, draw a picture of the silane molecule your group is using, (middle) Draw your silane molecule after it reacts with water, (right) Draw a section of the glass slide and your silane molecule after the condensation reaction in the oven. These examples may be noncanonical.

The students worked collaboratively, using pre-built physical models of the precursors which were used as manipulatives and to help visualize the reactions that were occurring.(Figure 6)



175 Figure 6. (left) Molecular model kit that was available to students in lab. (right) an example of a student's drawing of the molecular structure of their modified glass slide.

Pedagogically, the intention was for students to equate the macroscopic processes (i.e., doing and observing) with submicroscopic models, focusing students on the molecular level and giving TAs an opportunity to adjust and/or reinforce students' understanding of the reactions as they were occurring 180 and reducing the gap between the macroscopic and submicroscopic levels. Additionally, these pause and reflects occurred in sync with the actual processes in the experiment so students were modeling what they were doing while they were doing it (Figure 7). While the functionalization of the slides was expository in nature (i.e., instructor defines the topic and the procedures, and the outcome is predetermined)<sup>58</sup> we anticipated that closing the gap between the macroscopic and submicroscopic 185 levels in students' thinking would allow them to "see" the functional groups on the surface of the slides, and in their analysis and lab reports, to construct explanations that related the structure of the functional group to their observations.



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Figure 7. Schematic diagram of the procedure used to functionalize the slides and the “pause and reflects” embedded in the experiment.

190 The second part involved students collecting data on the interactions of water and of heptane with the modified surfaces of the slides. This phenomenon, known as wettability, refers to the ability of a liquid to maintain contact with a solid surface, caused by intermolecular interactions when the two are brought together. Since most students are already familiar with water beading on or “wetting” surfaces (e.g., rain on a waxed car or water pooling on a sidewalk), wettability is readily understood and embraced by students.<sup>59,60</sup> It is also significant in material sciences making its use relevant as a 195 laboratory process. Additionally, with ready access to and increasing resolution of smartphones cameras, clear and compelling observations of liquids interacting with surfaces can be recorded and further quantified using contact angle measurement, a well-established analytical technique.<sup>61-64</sup>

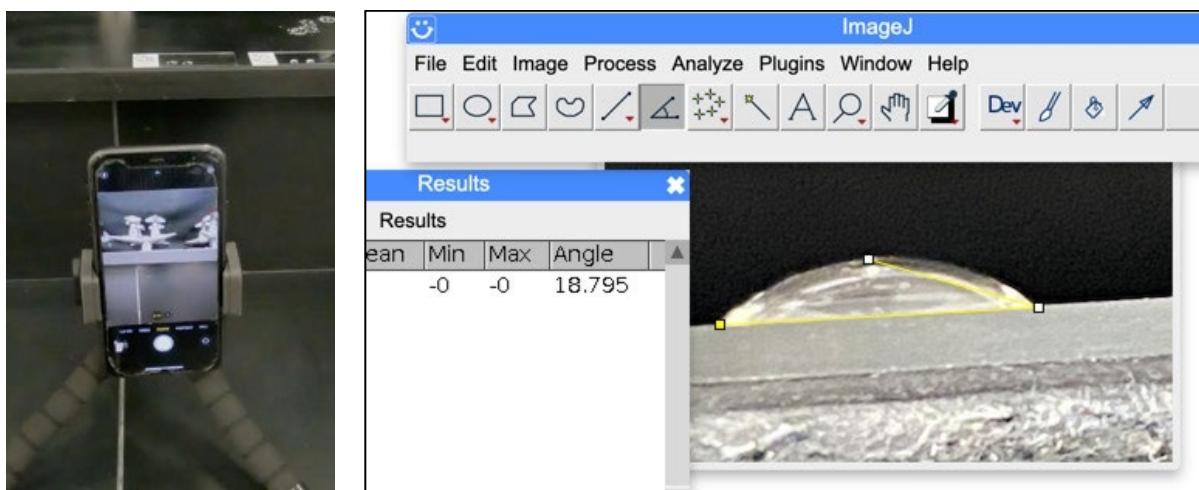
200 Armed with their own models of the molecular structures involved in the lab and the visual and numeric data of the interactions, students then engage in causal mechanistic reasoning in constructing explanations for their observations.

#### Experimental Procedure

205 **Part 1: Producing the functionalized slides.** Students were directed to work in pairs and with another group to conserve materials and time and to increase collaboration among students. The lab originally used three different alkoxy silanes: 3-(trimethoxysilyl)propyl acetate, 3-aminopropyltrimethoxysilane (APTMS), and octyltrimethoxysilane (Figure 2). But, after the first iteration in the Fall of 2023, the APTMS was dropped (the reason for this change is discussed in the Supporting Information). Students were instructed to mix pre-measured 500 $\mu$ L aliquots of their chosen alkoxy silane in the fume hood with 40mL of deionized (DI) water in polypropylene Coplin jars and to place two standard Corning type II soda-lime glass microscope slides in the capped jar and leave it for 10 minutes. The slides had a frosted end, were taken directly from the box, and labeled with pencil. The treated slides were then rinsed with DI water and placed in an oven that was pre-heated at 120°C. After 15 minutes, students removed, cooled, and shared slides so that all groups had one of each type of modified slide. Students also collected a clean untreated slide.

215 **Part 2: Characterizing the functionalized slides.** As a reference point, students took a picture of a water drop hanging on the tip of the micropipette. This provided practice using their smartphones

cameras and focused their attention to the appearance of the water drop when it was not interacting with a surface. To characterize the slides, students used micropipettes set at 30 $\mu$ L and placed two drop of DI water, 1cm apart, on each slide and then took profile pictures of the drops on the surfaces 220 with smartphone cameras. In the profile, the surface of the slide is horizontal and the left and right edges of the drop are visible and in focus (Figure 1). For better stability, students used small smartphone tripods with the slides set on raised surfaces( Figure 8). Crow *et al.* have reported 3-D printed set-ups for contact angle measurements,<sup>65</sup> and both Zou *et al.* and Wanamaker *et al.* have recently described easy-to-assemble contact angle measurement setup,<sup>66,67</sup> but we found the tripods 225 were cost effective and functioned well for a large scale lab. Students then measured the half angle of the drops from their drop profile pictures using the web-based version of *ImageJ* (Figure 7). While not as commonly used as other methods for measuring contact angle, half angle, the angle between the glass surface and the line drawn between the edge of the drop and the top of the drop, has been shown to give acceptable values if the contact angle is less than 90°.<sup>68</sup> Additionally, since students were not 230 asked to develop a mathematical relationship between surface structure and contact angle and the differences in contact angle between the various surfaces were significant (see results), using the simpler method to characterize the surface was sufficient for the needs of the experiment.



235 Figure 8. (left) Cell phone camera set on a tripod to take profile pictures of water drops on the functionalized slides. (right) Screenshot of *imageJ* software being used to measure the half angle of a water drop on an untreated slide .

As a final piece of data to consider in reasoning about liquid-surface interactions, students removed the water drops, placed a drop of heptane on each slide, took a picture from above (as the contact angle was too small to record), and described its appearance.

**Part 3: Analyzing and Interpreting Data.** As a prelude to analyzing the differences between the

slides, students were asked to describe the difference in appearance between the drop on the untreated slide and the drop on the micropipette tip (Figure 9), and then to explain the differences using molecular structure and IMFs. This is consistent with the use of contrasting cases to scaffold student thinking about mechanisms.<sup>69</sup>

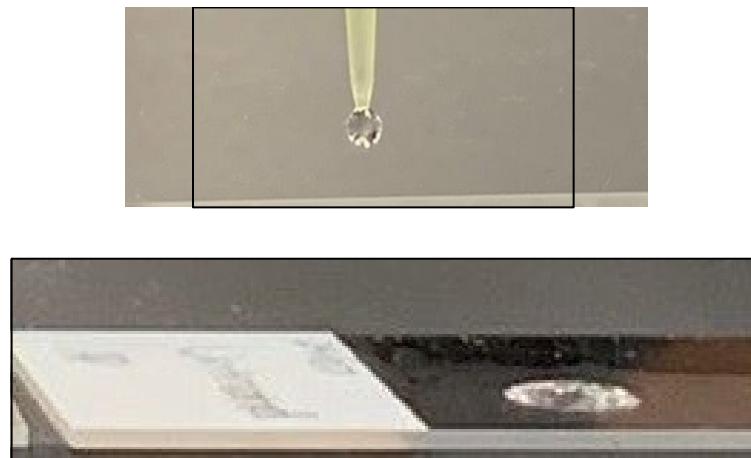
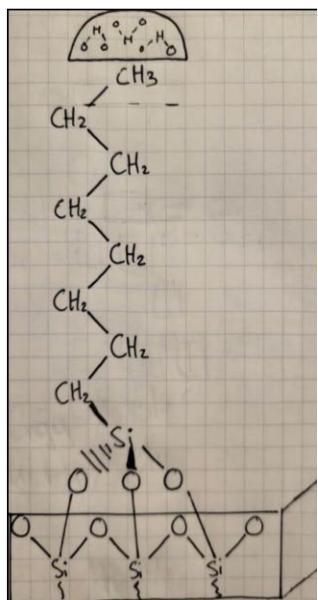
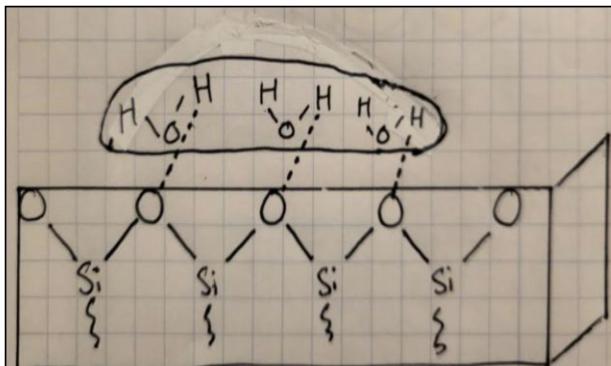
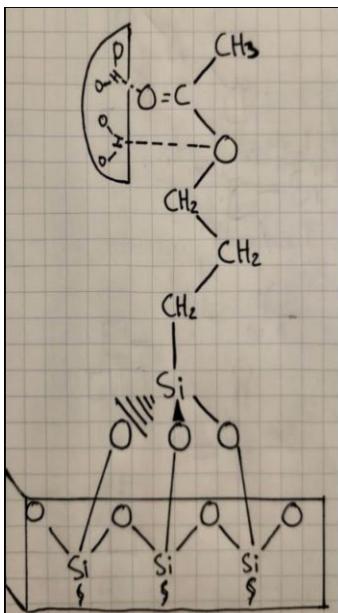


Figure 9. (top) picture of drop of water on the tip of the micropipette and (bottom) drop of water on the untreated glass slide from a consenting student (Sum24\_012).

Students then moved on to think about the functionalized slides. They were asked to consider and compare the polarity of the molecules on the treated slides as well as on the untreated slide, and the IMFs they believed were present between the water drops and the surfaces. They were then asked to complete drawings that modeled the IMFs that they proposed were present between the slides and the water (Figure 10), and to explain the cause of the differences between the half angles of the water drop on each slide. Finally, students were asked to explain why the heptane drops interreacted differently with the surfaces compared with the water drop.



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Figure 10. Example of student (Sum24\_010) response to the prompt to complete drawings that modeled the IMFs between water and the surface structure of the slides. Drawings may not be canonical.

## HAZARDS

Reagents used in this experiment include 3-(trimethoxysilyl)propyl acetate, octyltrimethoxysilane and *n*-heptane. Trimethoxysilanes are toxic if inhaled or swallowed and also skin irritants.<sup>70,71</sup> Proper protective equipment such as gloves, goggles and proper lab attire should be worn when handling the trimethoxysilanes. We recommend premeasuring the trimethoxysilanes into closed Eppendorf tubes that are stored and used by students in a dedicated fume hood with a waste container for emptied Eppendorf tubes. The hydroxylated form of both alkoxy silanes are irritants but are not toxic. Solutions containing the silanols should be collected and disposed of properly. When the alkoxy silanes are covalently bonded onto the slides by heating, they have no safety hazards so long as the slides do not break.

Heptane is flammable and should be kept away from any ignition source. It is a skin and eye irritant and may be fatal if swallowed. Proper protective equipment such as gloves, goggles, and proper lab attire should be worn when handling heptane. We recommend providing students with small quantities in closed reusable containers to reduce the risk of spillage and waste.

## DATA COLLECTION

1350 students completed the lab during the Fall 2023, Spring 2024, and Summer 2024 semesters. 445 students completed the lab and consented to have their lab reports accessed through the learning

management system (LMS) in compliance with the university's IRB (ID# 2018-1323). Of these, 225  
275 were randomly chosen for analysis. All quotes, photographs, and drawings in this report are from  
consenting students.

## RESULTS AND DISCUSSION

### Experimental Results

The laboratory procedure to functionalize glass slides produced surfaces with distinct responses to  
280 water droplets as observed in the profiles of droplets on the slides (Figure 11). The glass slides are  
Corning<sup>©</sup> type II – Soda-Lime glass, which contains hydroxyl groups in the range of 150-400 ppm.<sup>72</sup>  
This provided reactive sites for the functionalization of the slides with trimethoxysilanes.<sup>46,51,73</sup>

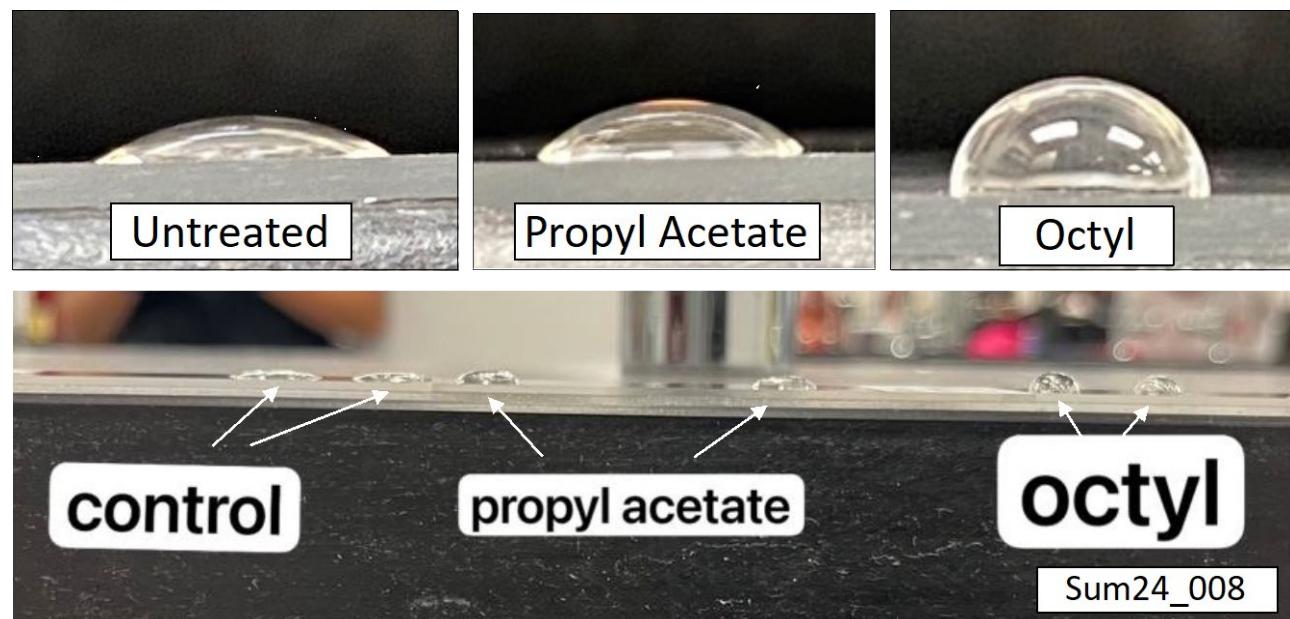


Figure 11. (top) Profiles of 30 $\mu$ L water droplet on untreated and treated slides produced by the authors using the laboratory procedure described in the paper. (below) Profile photograph from a student lab report. Control refers to the untreated glass slide.

285 Over 95% of students were successful in photographing and measuring half angles of water drops on their slides and over 85% measured and reported half angles that were consistent with expected trends (untreated<propyl acetate<octyl). These results were consistent over the three semesters (Figure S-19). A paired-samples t-test was conducted on student-measured half angles. A significant difference was found between the water drop half angle on the three surfaces (Supporting  
290 Information): the untreated slide ( $M=15.1^\circ$ ,  $SD=17.2$ ) and the propyl acetate slide ( $M=30.9^\circ$ ,  $SD=11.6$ ),  $t(225)=13.8$   $p<0.001$ ; the propyl acetate slide and the octyl slide ( $M=41.8^\circ$ ,  $SD=13.3$ ),  $[t(225)=15.4$   $p<0.001$ ; and the untreated slide and the octyl slide;  $t(225)= 22.8$   $p<0.001$  (Figure 12)]. This suggests

that the experiment is reliable in producing half angle measurements that are different for the three slides which students can then use in constructing explanations.

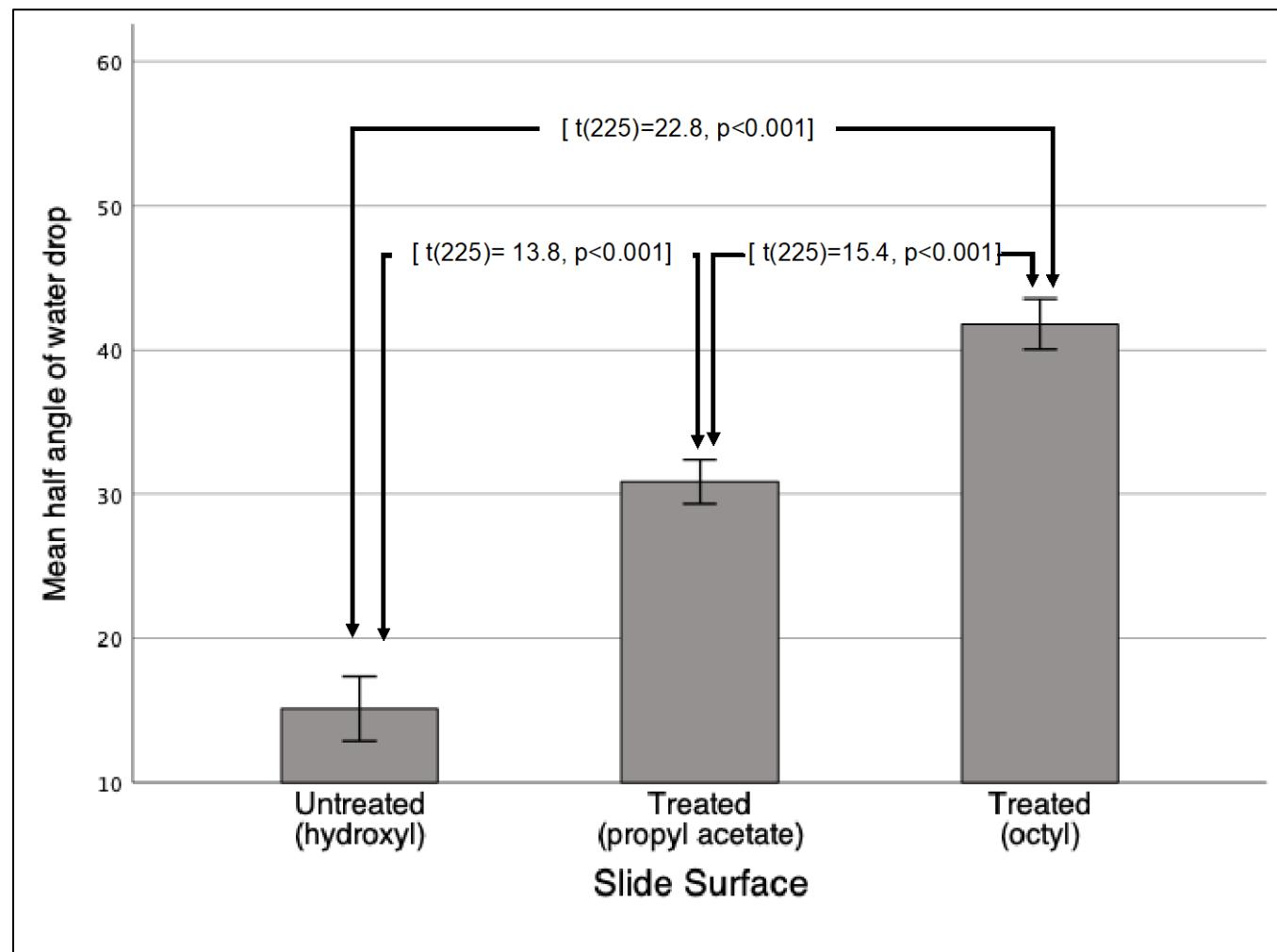


Figure 12. Mean contact half angles with 95% confidence interval of  $30\mu\text{L}$  water droplets on treated and untreated slides from consenting students' reports ( $N=225$ ). Paired samples t-test values are given at the top of the graph for the three pairings suggesting the experiment produces measured half angles that are significantly different from each other.

When students added a drop of heptane to each of the slides it was not possible to photograph the drop profile and therefore not possible to measure contact half angle. This was because the IMFs within the heptane drop were too small. Students were therefore instructed to take pictures from above (Figure 13) and to describe the appearance. Student pictures showed spread-out drops of heptane and most students described the appearance as spread out without distinct difference between the three different slides.



Figure 13. Photograph of a  $30\mu\text{L}$  drop of n-heptane on surfaces of (left) octyl treated, (middle) propyl acetate treated, and (right) the untreated slides demonstrating the similarity of spreading for all three slides. Photo taken with cell phone from above.

Student results are consistent with the concepts of molecular structure, polarity, and

310 intermolecular forces. If we consider the molecular model of the surfaces of the three slides (Figure 14), the untreated slides (Corning<sup>©</sup> type II – Soda-Lime glass) contain hydroxyl groups on their surface that provide sites for hydrogen bonding with the water molecules in the drop. This adhesive force competed with the cohesive force of the hydrogen bonding between water molecules within the water drop, causing the low contact half angle of the untreated slide ( $M=15.1^\circ$ ). The slide treated with the 315 octyltrimethoxysilane formed functional groups of eight-carbon chains on its surface with low polarity and weak attraction to the highly polar water molecules in the drop. Thus, the hydrogen bonding within the water droplet is significantly stronger than the dispersion forces between the alkyl functional group and water molecules , so the drop retains its spherical shape and a higher contact half angle ( $M=41.8^\circ$ ). The contact half angle for the slides functionalized with propyl acetate ( $M=30.9^\circ$ ) 320 can be explained by the presence of a polar ester group at the end of the propyl group with a dipole moment between 1- 2 Debye, depending on the environment,<sup>74</sup> and providing sites for hydrogen bonding to water molecules.<sup>75</sup> While the surfaces of the slides are likely more complex and 325 heterogeneous than implied here, as an introductory lab to IMFs and CMR, the idealizing of the functionalized slides and their interaction with water droplets is highly effective in fostering student learning. Additionally, the lab provides students with findings to stimulate additional questions about the molecular surface and its interaction with various substances (see Laboratory Extensions).

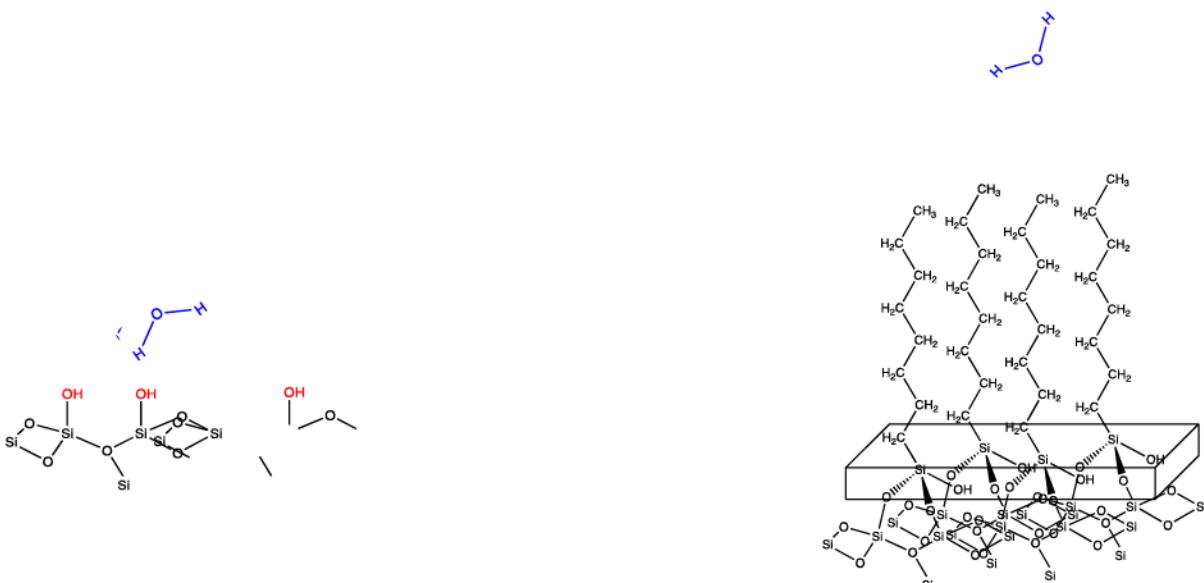


Figure 14. Schematic diagram of the possible interaction of the water with the three surfaces of the slide. IMFs are drawn as dotted lines. (left) the untreated slide with hydroxyl groups hydrogen bonding with water molecules, (middle) the propyl acetate slide with the ester group hydrogen bonding with the water molecules, and (right) the octyl treated slide with the alkyl groups forming dispersion forces with the water molecules. The diagrams are idealized realizing that the surfaces are likely more complicated than drawn.

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### Student CMR Responses

In their analysis and discussion, students consistently combined macroscopic and submicroscopic writing in describing and explaining their results, providing evidence of learning related to IMFs. When 335 asked to explain the difference between the water drop on the pipet with the drop on the slide, one student writes:

"The water drop on the micropipette was a lot rounder and sphere like while the water drops on the untreated glass was spread out, not very round and more flat like *[sic]*. This was due to 340 intermolecular forces and molecular structure because the drop from the pipette had high cohesive forces with the water. It was more spread out on the glass because there were stronger adhesive forces with the glass surface.... The water molecules were attracted to the surface causing it to pull outwards." (Sum24\_006)

Or as another student writes:

"When the water was dropped on a glass slide, it didn't form a round bead. This happened 345 because the glass has silanol groups on its surface, which have a strong attraction to the water molecules through hydrogen bonds...making it spread out and flat." (Sum24\_008)

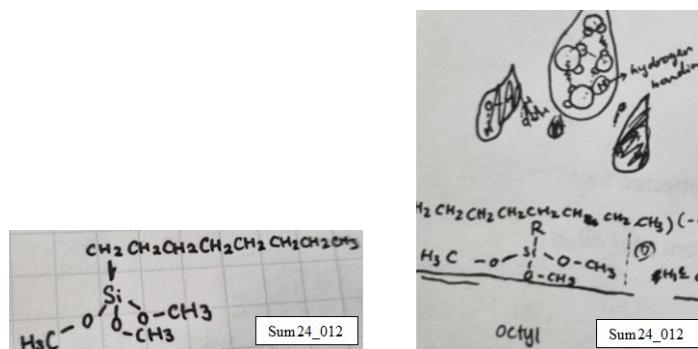
In both these responses, explanations move from macroscopic evidence (i.e., the shapes of the water droplets) to a scalar level below (e.g., silanol groups, molecules, and molecular structures) which references their properties (e.g., attractions and forces), and how these properties are relevant to the 350 phenomenon (i.e., the strong attraction makes the drop spread out); the characteristics of CMR.<sup>2</sup>

When asked to explain the differences between the droplet half angles on the three slides, responses typically continue to follow CMR as seen in the following portion of a student's response:

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Octyl silane has the biggest average drop half-angle out of all samples.... This is due to polarity and intermolecular forces present in each tested silane. Octyl silane only has dispersion intermolecular force acting upon it due to its hydrocarbon chain, and thus has the biggest half-angle out of all...(Sum24\_012).

Whose drawings were consistent with their argument (figure 15).



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Figure 15. Student Sum24\_012 drawings in response to the prompt to draw the structure of the starting material (left) and the interaction between the functional group on the slide surface and the water drop (right).

Or this student whose writing holds both the evidence and argument through multiple steps of their explanation:

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"The first glass slide, the Octyl chain had a weak reaction with the water due to its nonpolar surface. This led to a more spherical droplet and a larger half-angle. The bonds formed were the weakest being dispersion only. The second slide, the Propyl Acetate reacted moderately with the water due to its polar nature and this led to a little more spreading and slightly decreased half-angle. The bond formed here was dispersion and dipole-dipole due to the polar surface. This bond is stronger than dispersion only and the Octyl chain. Finally, the untreated surface had the best reaction to the water droplet as it formed the strongest hydrogen bonds. This led to the water spreading a lot and the smallest half-angle due to the polar surface and the strong hydrogen bonds." (Sum24\_009)

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While not all students expressed canonical causal mechanistic explanations or described IMFs normatively, most students were successful at providing explanations of the phenomenon of drop half angle on the glass surface using intermolecular forces. A more in-depth analysis of students' conceptions of IMFs is the topic of a future report.

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Finally, students were asked to explain the difference between the water drops on the slides and the heptane drops on the slides. While some students were successful at describing and explaining the

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greater spread of the heptane on the slides as due to the weak dispersion forces in the heptane drop and the low cohesion, this was not a common response and warrants continued analysis.

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### LABORATORY EXTENSIONS

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We used this experiment to strengthen students' understanding of IMFs using causal mechanistic reasoning of a very concrete phenomenon. The procedure was highly structured in modifying and characterizing the glass, but we can see it functioning in a more inquiry or CURES structured environment as well. Silanes have a rich history in chemistry education dating back to 1946 for their importance in polymer chemistry,<sup>76</sup> and more recently, surface chemistry.<sup>77</sup> While we used only two trimethoxysilanes and type II soda-lime glass slides for this experiment, there are a large number of commercially available silanes and silica surfaces with which to explore physical and chemical properties at various levels of the undergraduate chemistry curriculum. Additionally, we used one of the simpler methods of characterizing the slide surfaces—drop half angles from a cellphone picture measured with *ImageJ*—but there are many more sophisticated methods of collecting and analyzing drop contact angles.<sup>59,62,65–67,78–80</sup> Even in this experiment there are a number of avenues to explore concerning the modification of the surface (e.g., physical structure of the glass, heterogeneity of the surface, characterizing the surface with more advanced analytical techniques, stoichiometry of the reactions, thermodynamics of the surface interactions,<sup>78</sup> and robustness of the functionalized surface).

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We are aware that the environment of the slides and the water drop is likely more complex and heterogeneous than suggested here<sup>81</sup> and we are cognizant of the concern put forth by Talanquer of distortion and derandomization in developing mechanistic explanations.<sup>7</sup> But we believe that as an introductory lab to IMFs and causal mechanistic reasoning, it is highly effective in fostering student learning. Additionally, the lab provides students with findings to stimulate additional questions about the molecular surface and its interaction with various substances.

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### CONCLUSION

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We have developed a well-structured, robust experiment in which students use alkoxy silanes to produce functionalized glass slides and then characterize those slides by measuring half angles of water drops on the slides. Students use the core chemistry ideas of IMFs and molecular structure to construct causal mechanistic explanations of the differences in the water drop shape on the slides.

Students extend their understanding of IMFs by comparing how both water and heptane interact with the slide surfaces. Over three semesters and more than 1300 students, data was reliable and provided observable and empirically valid evidence that students used in their explanations. By scaffolding the lab with pause and reflect stops, the activity allows students to develop richer understanding of the submicroscopic structure implicit in the reactions and how their properties impact the macroscopic interaction between different surfaces and liquids. This laboratory activity opens a number of additional avenues for undergraduate lab study of IMFs, surface properties, and functionalization experiments, providing authentic experimentation and three-dimensional learning.

## ASSOCIATED CONTENT

### Supporting Information

The Supporting Information is available on the ACS Publications website at DOI:

10.1021/acs.jchemed.XXXXXXX. [ACS will fill this in.]

File containing the complete laboratory procedure for students, instructor's notes, grading rubric, components of 3-dimensional learning, and statistical analysis of student data. (DOCX)

Slide deck of accompanying lecture to the experiment. (pdf)

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## ACKNOWLEDGMENTS

We acknowledge the support of Thomas Rickhoff, Lisa Merdjane, and Christian Berger in their careful preparation of the lab materials for these labs, the CER community at UIC for their

435 encouragement and their insights into the teaching lab and student learning. Work was also supported, in part, by NSF grant (DUE-2111446).

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