Fats' love-hate relationships: a molecular dynamics simulation and hands-on experiment outreach activity to introduce the amphiphilic nature and biological functions of lipids to young students and the general public

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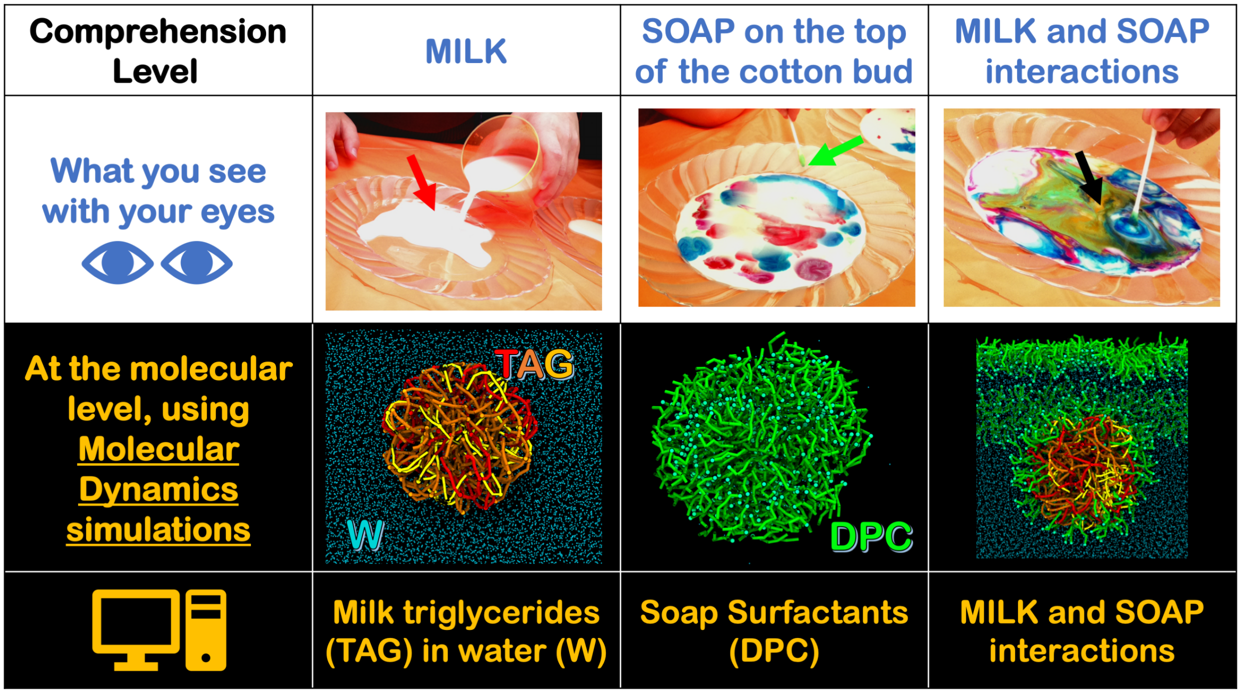
ABSTRACT

Lipids are fundamental components of biological organisms and have important applications in the pharmaceutical, food and cosmetics industries. Thus, it is important that young students and the general public properly understand the basic properties of lipids and how these relate to their biological and industrial roles. Here, we use molecular dynamics computer simulations and a simple, safe and inexpensive popular hands-on activity, to communicate to participants why and how lipid molecules play a fundamental role in all living organisms and in our bodies. The activity is called "Fats' love-hate relationships", to highlight how the different parts of amphiphilic lipids interact with water. This "love-hate relationship" is vital to the biological functions of lipids and drives the formation of lipid structures that can be visualized at molecular scale with the computer simulations. The participants were encouraged to investigate the interactions between milk lipids and soap surfactants, creating beautiful complex artwork that they could then take home. The hands-on

activity was accompanied by a video of a molecular simulation that illustrates milk-soap interactions at a molecular scale and helps to explain how the amphiphilicity of lipids creates the beautiful artwork at a molecular level. The outreach activity has been performed in science festivals and in classrooms and has been well received by participants of all ages with multiple learner comprehension levels (primary and secondary school students and general public). By combining molecular simulation, explanations of the amphiphilic structure of the lipids, and an engaging hands-on activity, we explained how lipids interact with water and surfactants, and inspired discussions on the link between the structure of the lipids and their biological function, namely, their structural and protective roles as a key component of cell membranes.

GRAPHICAL ABSTRACT



KEYWORDS

General Public, Elementary/Middle School Science, Public Understanding/Outreach, Biochemistry, Hands-On Learning/Manipulatives, Lipids, Molecular Properties/Structure, Computer-Based Learning.

INTRODUCTION

Lipids are one of the four major classes of biomolecules, which are prevalent in all living organisms.[1] Based on their structures, lipids fall into eight categories: fatty acyls, glycerolipids, glycerophospholipids, sphingolipids, saccharolipids, sterol lipids, prenol lipids and polyketides.[2] As shown in Figure 1, typical lipid structures usually contain either long hydrocarbon chains or fused hydrocarbon rings, so they are hydrophobic or amphiphilic. The main functions of lipids include membrane formation (glycerophospholipids, sphingomyelin and sterols), energy storage (fatty acids and triglycerolipids) and signaling (some sphingolipids and saccharolipids).[3] Besides their biological functions, lipids have been widely used in the pharmaceutical, food and cosmetics industries, as transdermal excipients, nutritional supplements and emulsifiers.[4] Moreover, there are some new emerging applications of lipids including biodiesel extraction from plants as renewable energy[5–8] and formulation of new nanomedicines using solid lipid nanoparticles or liposomes[9,10].

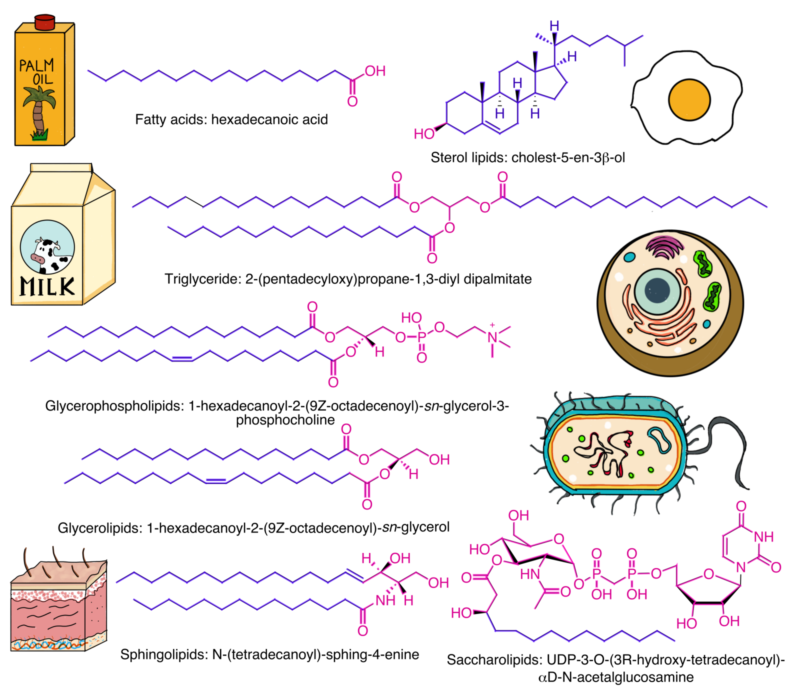


Figure 1. Representative lipid structures. The hydrophilic part of the molecules is highlighted in magenta, and the hydrophobic part in blue. Next to the lipid structures we present some examples of food or systems which have those lipids in their composition. Specifically, we show palm oil for hexadecanoic acid, eggs for sterol lipids, milk for triglycerides, cell membranes for glycerophospholipids, bacteria membranes for glycerolipids and saccharolipids, and skin membranes for sphingolipids.

Despite their important biological functions and widespread industrial applications, the general public tends to have a negative impression of lipids, especially fats. Of course, there are some exceptions to this such as omega-3 fatty acids which have been widely publicized for their benefits associated with healthy aging;[11] while the negative roles of fats are more specifically associated with saturated and trans fats.[12] However, this distinction is not always clear to the general public, with the public's overall negative impression due to the strong emphasis placed by the press and social media on dangers to health, especially obesity and cardiovascular diseases.[13,14] According to one of the largest global studies published on the public perception of fats, more than half (59%) of 6,426 participants from 16 countries believe fats should be avoided from diet.[15] This study shows that the general population has a significant lack of knowledge or biased understanding of fats. Therefore, it is necessary to explain the fundamental importance of lipids to the public and engage school students on this topic.

To understand the significance of lipids it is important to introduce one of the key properties of lipid molecules: *amphiphilicity*. In Figure 1 we have highlighted the *hydrophilic* part of the lipid molecules (the part that interacts favorably with water) in magenta and the *hydrophobic* (unfavorable interactions with water) parts in blue. The combination of a hydrophilic head group and hydrophobic tails allows amphiphilic lipids to *self-assemble* into structures which are vital to the roles played by lipids. Amphiphilic molecules interact with water in a complex way. The polar head group interacts strongly with water which solvates it, while the hydrophobic tail interacts weakly with water. The amphiphilic character of these molecules drives self-assembly of the lipids when they are in contact with water, with the polar regions interacting preferentially between themselves and water while the hydrophobic tails bundle together to minimize contact with water. This is the driving force for self-assembly into lipid bilayers which are the main constituents of cell membranes, and soap surfactant micelles (as shown in the right panels of Figure 2).

Since the molecular concept of amphiphilicity is difficult to understand for the general public, we designed an educational activity named as “Fats’ love-hate relationships”, combining a popular hands-on experiment with molecular dynamics (MD) simulations, to demonstrate the interaction between lipids and water experimentally and *in silico* at a molecular level. To the best of our knowledge, this is the first activity combining MD simulations with practical outreach and classroom activities.

To explain amphiphilicity qualitatively, we describe the interactions between lipids and water as a “Love-hate relationship”. Personifying the interactions of lipid molecules in this way can make the underlying ideas of amphiphilicity more relatable and easier to grasp for participants since there is no need to have a detailed prior understanding of the molecular structure of lipids and their polarity characteristics.

The key aspect of our educational activity is that it incorporates MD simulations to explain the concepts of amphiphilicity and self-assembly in an intuitive way. MD is a computer simulation technique that employs Newtonian mechanics to compute the time evolution of atoms and molecules, using as input the interactions between atoms[16]. Since its development in the 1950s, MD has become increasingly widespread in biochemistry, biophysics and material science. It can be used to investigate the three-dimensional structure of proteins, the interaction between different macromolecules, or the penetration of nanoparticles in cell membranes. The importance of MD was recognized by the award of the 2013 Nobel

Prize in Chemistry.[17] As MD has become an important tool in research, there are attempts to introduce it into chemistry education for students that specialize in chemistry or biology at the college level.[18–27] Most MD education is directed towards undergraduate students. This is likely connected to the need to understand the complex theories and equations behind it.

We believe that MD can be used more widely to engage the general public with molecular processes, since it provides vivid graphical images and videos which are easy to understand, especially when connected to macroscopic observations. In this activity, we used the hands-on activity to allow participants to investigate the interactions between the water and triglyceride lipids in milk with soap surfactants, inspired by popular science activities called 'colors on the mooooove'[28] and 'milk rainbow'.[29,30] We used MD here as a vehicle to explain lipid-water interactions and to rationalize macroscopic observations of self-assembly in milk-surfactant-water mixtures. In addition, the practical activity was accompanied by a discussion and a series of posters highlighting the role of lipids and how their "love-hate relationship" with water gave rise to the observed behavior. Since the activity is simple, safe, inexpensive and easy to perform, it is suitable for presenting to the public in science festivals, or to students of different ages in a classroom. It can also be easily repeated at home to impress family and friends. The specific learning objectives are:

- Identify common substances containing lipids and their applications;
- Define the concept of amphiphilicity of lipid molecules and explain where and why it is important;

- Compare macroscopic observations of the milk experiment with the MD simulation video of soap-milk lipid interactions;
- Recognize the value of MD simulations as a tool for scientific studies at a molecular level.

PRESENTING THE HANDS-ON ACTIVITY

Materials

Here we list all the materials for this activity:

- Experimental consumables: different types of milk (whole milk, soya milk and skimmed milk), washing-up liquid (dishwashing liquid), cotton buds, food coloring (or watercolor) solutions (1:4 mix of food coloring to water), disposable dishes (to hold the milk), plastic pipettes (for dropping the food coloring onto the milk surface), watercolor paper of different shapes (for printing the artwork from the milk surface), and permanent markers (for leaving notes and feedback).
- Computer simulation: a display and a device (e.g. a laptop, a tablet or a smartphone) to play the Video S1.
- Other materials: bins for waste dishes and milk, kitchen rolls for wiping up spilt liquids, posters and flyers (see the Supporting Information).

Performing the activity

We began the activity with a brief introduction to lipids, initiated by several motivating questions for the audience:

1. Where can we find fats in everyday life?
2. What are the functions of fats?
3. How can fats perform these functions?

To gather answers to the *first question* above, about the sources of fats, we performed an observational exercise, where the audience was asked to think and list the substances in their everyday life which contain fats. To stimulate the participants to think about fats, examples of lipid containing products were shown to the audience. These included both products commonly referred to as fats, such as food products including milk, butter and cooking oil and products less commonly associated with fats such as detergents and cosmetics. In response to the *second question* about fats' functionality, the audience was encouraged to think about what sorts of roles the fats played in these products and what determines the different roles of fats. Finally, we addressed the *third question*, the basic amphiphilic nature of the molecular structure of lipids was introduced, explained via the metaphor of "love-hate relationships" with water, as shown in Figure 2. The personification of lipid molecules in a "love-hate relationship" was found to be a useful tool to introduce amphiphilicity to participants with no or limited prior chemistry knowledge and enabled participants, especially young children, to immediately start to think about how they would arrange themselves if they were lipid molecules, e.g. by moving around and copying the cartoon in Figure 2. This illustrates the potential that personification has in science education, particularly to explain difficult concepts, as has been previously explored by Wallon and Brown.[31]

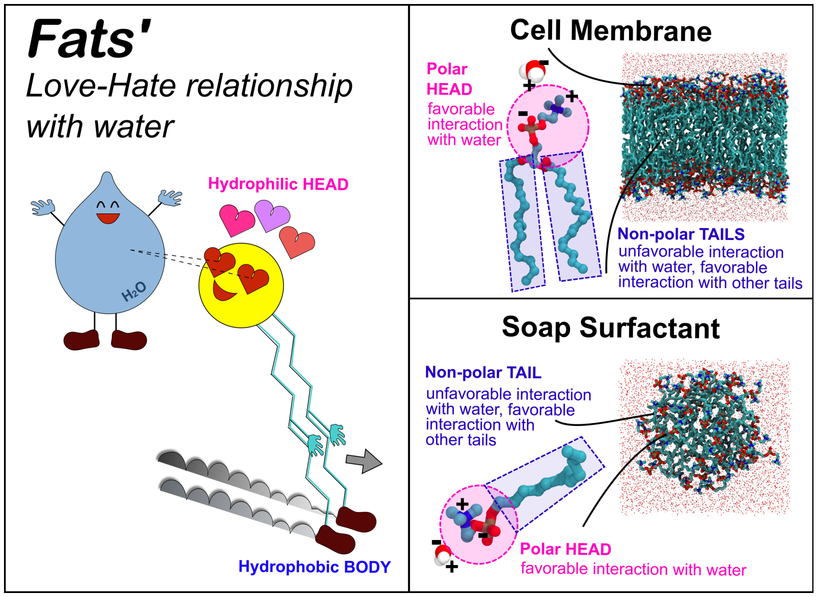


Figure 2. A schematic (cartoon-style) representation of "Fats' love-hate relationships" with water (left-hand side). The cartoon depicts the fat molecule as a person with two different parts, a hydrophilic, water loving "head" and water hating "legs" which represent the hydrophobic tail groups of the lipid. This visual metaphor makes the amphiphilic properties of lipid molecules easier to understand for people with no prior knowledge of molecular structure, polarity or hydrophobicity. The role of the lipid amphiphilicity or 'love-hate relationships' with water, in forming the structures of cell membrane bilayers and surfactant micelles is then shown (right-hand side).

After explaining the amphiphilicity concept, the hands-on experiment was carried out to show how fats interact with each other and with water, specifically our activity focused on milk lipids and soap. Figure 3 visualizes four key experimental steps from left to right. Firstly, milk was poured into a shallow dish (Figure 3A). Participants were encouraged to choose different types of milk (soya, skimmed or whole milk) for comparison. This also avoids any potential problem for people with allergies to lactose or soya. Secondly, several drops of food coloring or watercolor solutions were pipetted onto the milk surface to produce small, concentrated patches of different colors (Figure 3B). For young children, it was necessary to explain how to use plastic pipettes to suck up and release the solutions. Thirdly, a small drop of washing-up liquid was loaded onto the tip of a cotton bud (Figure 3C). Finally, the cotton bud tip was placed on to the surface of the milk, near or within the color drops (Figure 3D).

Results of the activity

As the tip of the cotton bud touched the milk surface, the color rapidly spread out in all directions, away from the cotton bud as the washing-up liquid interacted with the milk. The effects were different depending on the type of milk. The colorful patterns produced on the milk surface were then transferred to the watercolor paper, which served as a take-home souvenir to remind the participants about the activity and what they had learned. In addition, the participants took home flyers containing the experimental instructions (see dedicated section in the Supporting Information) for repeating the experiment at home.

SAFETY AND HAZARDS

All materials used are common household products and are non-hazardous. However, if splashed into eyes, the washing-up liquid may cause irritation. If this happens, contact lenses should be removed immediately and large amount of water should be used to rinse off the washing up liquid thoroughly for several minutes. People with allergies to milk or lactose should be reminded to use soya milk for the hands-on activities.

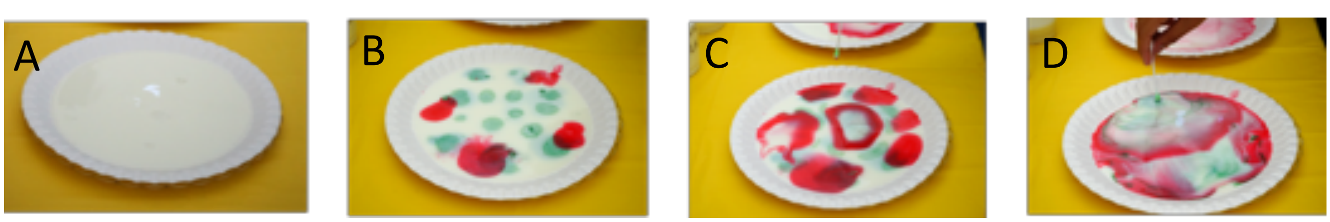


Figure 3. Four key experimental steps visualized by pictures taken during a science festival at Imperial College (Imperial Festival): (A) The milk, containing the triglyceride lipids and water is poured into a dish. (B) Drops of food colorant (red and green spots) are pipetted onto the milk surface. (C) A cotton bud tip containing washing-up liquid is touched on the milk surface within two of the spots of food coloring. The soap molecules are surface active. They adsorb at the interface, spreading on the surface of the milk, pushing the coloring as they move, and forming the final color patterns in (D).

THE MD SIMULATION

Following this simple experiment, a video explaining the main features of fats and a computer simulation of milk-soap interactions in water, was played to illustrate the molecular behaviour responsible for the spreading process which causes the striking macroscopic effect observed in the activity.

In the simulation, the milk was represented as a mixture of water and triglycerides (the most abundant lipids in milk[30]), namely tripalmitin (TPG), triolein (TOG) and trilaurin (TLG). Different degrees of saturation and chain lengths were chosen to represent the diversity of different lipids in milk (see Figure 4). The soap was represented by a common surfactant: dodecylphosphocholine (DPC).

Food coloring is made up of pigments diluted in a water-based solution.[32] Due to the very low concentration of the pigment molecules, they do not play a significant role in the interactions between milk lipids and soap, therefore we didn't include those molecules in our simulation model. Their role in the hands-on activity is to allow the public to visualize the interactions between milk and soap. In the MD simulation we can track the molecular behaviour of the different lipids just by representing the molecule with different colors.

MD simulations rely on the definition of a forcefield, a mathematical function of the positions of all the particles in a system, which defines the interactions between the particles and hence the potential energy of a system configuration. Depending on the degree of resolution of the molecules, forcefields can be classified as atomistic (every atom in a molecule is represented explicitly as a particle) or coarse grained (CG). In a CG forcefield, molecules are represented by fewer particles while maintaining some chemical specificity by combining atoms within functional groups or natural molecular subunits into a single particle. CG forcefields enable longer timescales to be reached, which is important to capture the behaviour responsible for many macroscopic observations. The milk-soap simulations were performed using the MARTINI forcefield,[33] which is widely used to model lipid membranes. More details on the forcefield are available in the Supplementary Information and in reference 33. In Figure 4 we show the MARTINI representations of the molecules used in our simulation and highlight how the underlying molecular structures of the molecules are represented in the MARTINI forcefield, namely by groups of atoms into single “beads” (represented by the colored circles in Figure 4). In the MARTINI model, each interaction site or “bead” represents roughly 4 non-hydrogen atoms and the models has been parametrized to reproduce the interactions of polar and non-polar groups with water. The different colors in Figure 4 highlight different particle properties as explained in the Supplementary Information.

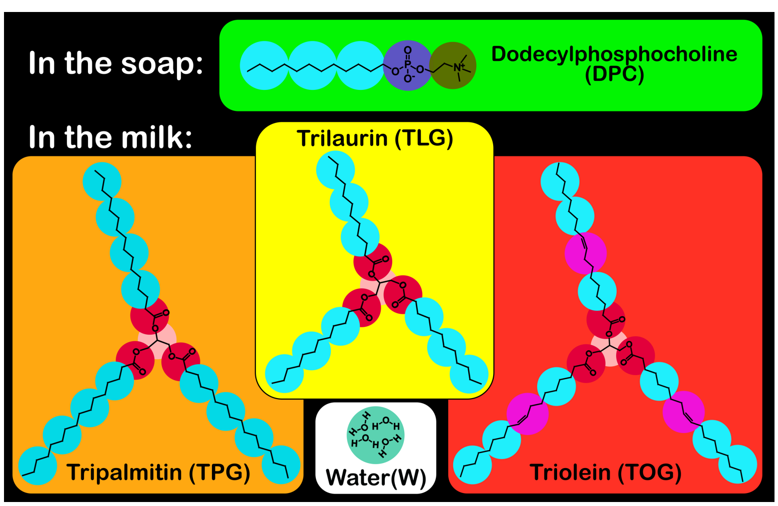


Figure 4. Modelling of soap and milk using MD simulations of coarse grained forcefields: DPC (soap), W (water), TPG, TOG and TLG (milk triglycerides). The groups of atoms combined to form each individual bead in the MARTINI forcefield are enclosed by the colored circles which represent the MARTINI beads. The color of the different beads corresponds to its description within the MARTINI forcefield as explained in the Supplementary Information. Each lipid molecule is drawn within a box, the color of which corresponds to the color of the molecule in the MD simulation video S1 and snapshots in Figure 5, *i.e.* light green for DPC, orange for TPG, yellow for TLG and red for TOG. The MARTINI water particle represents 4 real water molecules.

To provide a microscopic interpretation to the observations of the hands-on activity, an MD simulation was used to visualize the molecular self-assembly emerging from the water-lipid-surfactant interactions. A system was constructed consisting of a soap micelle, which was initially placed above the surface of our computational model of milk, which contains water and triglycerides. The soap micelle contained 500 DPC molecules and forms a spherical shape to minimise exposed surface area. The milk contained 10,306 MARTINI water particles, approximately equivalent to 40,000 real water molecules, and 50 molecules of TPG, 20 molecules of TLG and 30 molecules of TOG. Milk triglycerides in water cluster together, forming a spherical structure, which resembles the structure of a milk globule.[34] The initial configuration, composed of a total of ~15,000 particles, is shown in Figure 5A (left-hand side panel).

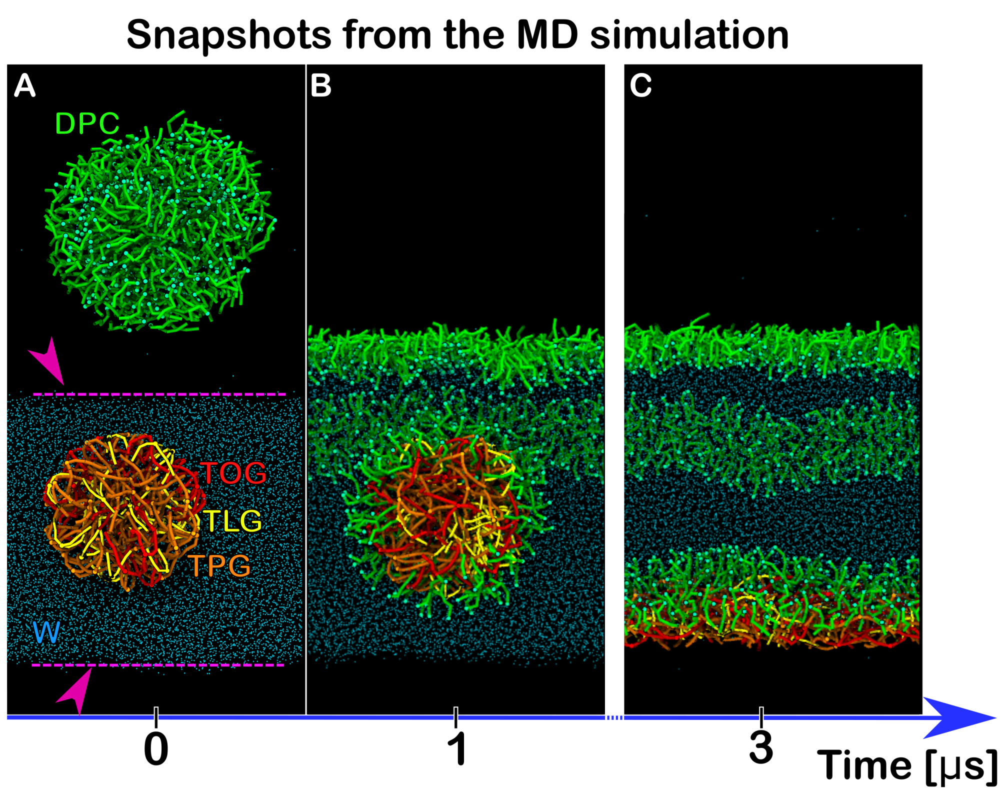


Figure 5. Three representative snapshots extracted from the MD trajectory. (A) Soap surfactant droplet (DPC) approaching the milk surface. (B) Interactions between soap (DPC) and milk (TOG, TLG and TPG) fats, forming a soap monolayer on the milk surface and a soap-milk micelle around the milk triglycerides. (C) The milk globule is destroyed, and the milk fats are carried to the interface lowering the interfacial surface tension. DPC soap surfactant is represented in green and different milk triglycerides in orange (TPG), red (TOG) and yellow (TLG). The head group beads are represented as a ball and the hydrophobic tails as sticks. Water in the milk is represented with light-blue dots. Magenta arrows point to the air-milk interfaces.

As shown in the simulation video S1, the surfactant micelle quickly approaches the milk surface and starts interacting with water and the milk lipids. Due to the strong interaction between the headgroups of DPC molecules and water, some of the soap lipids reorient on the surface, with the hydrophilic (“water-loving”) beads facing the water interface and the hydrophobic (“water-hating”) tails pointing away from the water, towards the air. This behaviour immediately illustrates the principle of amphiphilicity or “love-hate relationships” introduced in the previous parts of the activity. The amphiphilic interactions create a surfactant monolayer at the air-milk interface. However, the surfactants also interact with the lipids in the milk (Figure 5B, middle panel), leading to the destruction of the milk globule and the transport of the milk lipids to the milk-air interface (Figure 5C, right-hand side panel). The combination of these interactions drives the macroscopic effects observed in the experiment, creating a flow that drags the food coloring to move across the milk surface mixing different droplets, pushed out by the formation of the monolayer, and ultimately produces the colorful patterns which form on the surface. The formation of a lipid layer on the milk surface can also be experienced at the end of the experiment by dropping a small droplet of water from the cotton bud onto the milk surface after adding the soap. This water droplet will run on the milk surface, separated from the milk by the lipid monolayer. More details about the MD simulation technique and the set-up of this system are available in the Supporting Information.

DISCUSSION

The aim of this activity was to introduce the general public to the importance of lipids and to communicate how the amphiphilic molecular structure of many lipids is vital to their functions. The anthropomorphisation of lipids and the description of lipids' "love-hate relationships" to describe the interactions with water was found to be an effective way to introduce the molecular structure of lipids. Even young children that were not familiar with molecular structure or polarity were able to engage with the love-hate relationship idea and the cartoon image of Figure 2, many of them acting out the same pose and able to predict how they would arrange themselves as lipid molecules.

We exploited the power of computer simulation to reproduce the key microscopic interactions that are in play during the experiment. At each stage of the video showing the MD simulation, participants were asked to think about how the lipids' "love-hate relationships" were likely to affect the interactions between different components of the system and to predict how the system would evolve. The connection between the formation of a lipid monolayer on the surface of the milk in the simulation, and the movement of food coloring across the milk surface as soap was added during the experiment was then easily explained. Specifically, the formation of the soap monolayer at the air-milk interface explains how the contact with the detergent lowers the surface tension of the liquid so that the food coloring is free to spread across the milk surface. Due to the soap interaction with milk lipids, they rearrange onto the surface, keeping the food coloring moving and producing spectacular and artistic patterns onto the surface. The simulation also illustrated the power of molecular simulation, sometimes referred to as a "computational microscope",[35,36] to reveal the molecular interactions that are responsible for the observed macroscopic behavior. Participants were very excited by being able to watch the process at a molecular level and could appreciate the significance of computational simulation as a scientific technique.

To collect feedback from the participants, we encouraged them to write their comments on the final artwork produced at the end of the experiment. We collected a total of ~1000 artworks (examples shown in the Supporting Information, Figure S15) and all comments that we received were positive. We statistically analyzed the most frequently recurring keywords in the feedback and the results are presented in Figure S15. However, a limitation of this method is that measuring the occurrence of particular keywords expressing feelings or emotions about learning might not imply that the participants really learnt from the activity. Therefore, a questionnaire for participants to complete after the activity was also produced in order to acquire some feedback about the effectiveness of the activity and the MD simulations. The feedback questionnaire needs to be simple and effective and can be completed on a portable device, such as a tablet or a mobile phone, which can be presented for example with a google-form. An example is proposed in the Supporting Information and can be accessed via the web link: https://forms.gle/DNeMCkm36Wnjzarf7.

When demonstrated in classrooms, the feedback survey could include a practical activity where students are asked to draw on paper how lipid molecules would self-assemble in water. The activity would work well alongside basic lectures on chemistry and biology focusing on hydrophobic interactions and lipids. We believe that the video presented in here will be helpful for use in classrooms to illustrate, at a microscopic level, how lipid-water interactions work.

There are some limitations in our current implementation of the activity, which are related to the final visual effects and artwork transfer of the hands-on activity. We found that the transfer of the colorful patterns to paper to generate the artwork does not always work. First of all, the type of paper and color is crucial. We found that the best results were produced by using watercolor paper, due to its thickness and the rough surface, and quick-setting watercolors. Watercolor solutions need to be prepared in advance by properly mixing the paint with water to avoid precipitation. Secondly, we noticed that people often stirred the milk once the reaction slowed down, which destroyed the color patterns produced during the experiment. So, it is important to remind the audience not to stir the milk once the experiment is completed. Finally, compared to soya and almond milks, the use of cow's milk led to a faster reaction and more dissolved colors, due its higher content of fats. Although this makes very nice visual effects, we found that it is more difficult to transfer to paper.

CONCLUSION

In summary, we report an interactive outreach activity combining MD simulations with a simple hands-on experiment to introduce the amphiphilic nature of lipids, which plays a key role in their biological functions. The activity is designed for young students and the general public, with no previous scientific background. The activity is safe, inexpensive and easy to perform in science festivals as well as in classrooms. We have presented the activity a number of times at different events, including the Imperial Science Festival, Royal Institution Family Fun Day and as part of science demonstrations in schools around London (see the Supporting Information for a full list). We found that displaying the molecular mechanisms behind the practical activity via MD simulations helped the overall comprehension of the topic and to engage the audience. The notes written on the artwork used to collect feedback from young students and the general public indicated the positive outcomes of the activity. The simulations have allowed the key amphiphilic nature of lipids and the importance of this characteristic to their behaviour and biological function, to be introduced to the general public.

ASSOCIATED CONTENT

Supporting Information

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

The supplementary material includes the following contents:

Details on the MD simulation method and set-up; Preparation before the outreach activity and summary of previous demonstrations; Posters and flyers used for the realization and promotion of the activity; Stand photos; Activity feedback including the analysis of the frequency of keywords and feedback questionnaire; Picture of our designed T-shirt for the image contest we organized (DOCX)

Video S1 showing the computer simulation results (MP4)

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Notes

The authors declare no competing financial interest.

ACKNOWLEDGMENTS

We thank the Marie Curie Actions under the EU FP7 Initial Training Network SNAL 608184 for funding and stimulating researchers towards outreach activities. We also thank Imperial College London for organizing outreach activities within the institution. Special thanks to all the volunteers assisting with the realization of the activity in schools and science festivals: Zainab Ahmed, Marie Bachelet, James W Carter, Yu Han Chang, Siyuan Chen, Daniela Ciumac, Silvia Di Lecce, Gøran Svatland, Christian Jürgensen, Michal Kopytynski, Berardo Mario Manzi, Enrica Mazzon, Suhuur Osman, and Oliver Robotham. We also thank Dr. Xin Tang and James W Carter for helpful discussion and suggestions.

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