Janus Particles Exploration – Daniel Sinkovits

Purpose

This lesson is an exercise in making and evaluating predictions based on the outcome of a simulation. The context for these predictions is the cutting-edge soft matter research topic of patchy particles, which are colloidal particles that have patches of different interactions on them. Janus particles, having only two patches, are the simplest patchy particles. The relative simplicity allows students to observe the systematic change of structure as the particles are changed and also allows the students to make predictions that are both reasonable and not obvious.

Overview

The lesson begins with colloidal particles and purely attractive interactions, demonstrating the structures that form based on changing the temperature. Then, the students explore how a small attractive sector leads to dimers, and they explore how external properties affect the formation of dimers. Then, the students observe trimers and are challenged to make *specific* predictions of what they will see as the width of the attractive sector (Janus balance) is increased based on their understanding of the attractive interactions. Finally, their predictions are tested as they observe the structures that form at different Janus balances.

Student Outcomes

Students will be able to identify that temperature, concentration, and Janus balance affect the structures formed, and explain the general affect of each.

Students will be able to make a prediction of the structure that will form based on the attractive sectors on a particle.

Students will be able to identify discrepancies between their predictions and the actual outcomes.

Students will be able critically evaluate their reasoning behind the predictions based on the successes and failures of their predictions.

Illinois State Science Standards identified

- 11.A.4a Formulate hypotheses referencing prior research and knowledge.
- 11.A.3b Conduct scientific experiments that control all but one variable.
- 11.A.4e Formulate alternative hypotheses to explain unexpected results.

Time

Two 40-minute blocks of time.

Level

Junior High Science or High School Chemistry

Materials and Tools

Computers, one per group of 2–4 students

Internet access

Java installed

Handouts for first and second days

Computer linked to a projector for demonstrations

Preparation

It is sufficient preparation to work through the worksheet that the students are provided with.

Prerequisites

The students should have done activities before involving simulations or applets on the computer, so they are familiar with using a computer in class. They should also have learned what crystallization looks like on the molecular level. A simulation activity would be perfect for this. Finally, one of the questions mentions polymers, so it would be helpful if the students had been exposed to that concept recently.

Background

To succeed in this lesson, you need to follow directions carefully and make careful observations. You will be asked to make predictions, and it is important that they are as specific as possible.

Teaching Notes

First, introduce the concept of colloidal particles and Brownian motion as a guided discussion with the Java applet as a demonstration. The students can use the worksheet as a note-taking assistant. Then continue the demonstration and discussion through showing how attractive interactions cause the system to reach gas, liquid, and solid phases at different temperatures.

Then, group the students into pairs or triplets to work on the worksheet up to the point marked STOP. They will explore how a particles with a small attractive sector lead to dimers, and how temperature, concentration, and size of the attractive sector control this. You can call attention back to the front to ensure everyone is on the same page regarding how and why dimers form. Before the end of the first day, make sure that students have sufficiently specific predictions with drawings of what structures they expect to appear when the attractive sector is wider.

The next day, recap what was learned the day before: that attractive interactions lead to structure when the temperature is low, and that a small attractive sector leads to dimers, whose formation is affected by temperature, concentration, and the size of the attractive sector. Remind them that they saw trimers appear at higher Janus balances (wider attractive sectors) and that they made predictions of what other structures they will see if the attractive sectors are made even wider.

Then, let the students return to their groups to continue the worksheet. It directs them to observe the structures that form and has them compare to their predictions, looking for discrepant events—both structures that they did not expect and structures that they predicted that didn't form. They will also explore the large structures that form for Janus balance greater than 90 degrees, all the way up to full coverage of attractive interactions. Recap the lesson by emphasizing the value of making and testing predictions and soliciting what they learned from predictions that were not quite correct.

The last page of reflection questions can be done in class or as a homework assignment.

Assessment

Learning Objective	**Unsatisfactory**	**Developing**	**Satisfactory**	**Exceptional**
Identify how different factors affect structure (12–23)	Data not collected or no relationships explained.	All relationships are correct, but some explanations are insufficient.	All relationships are correct and all explanations make sense.	In addition, the explanations reference prior knowledge.
Make a prediction based on attractive sectors (26, 27)	No predictions made or only a vague prediction given in words.	Structures are drawn but make obvious errors (e.g. particles in non-bonding orientations).	Three structures are predicted and all particles are bonding correctly.	More than three structures are predicted and all predictions are sensible.
Identify discrepant events (28–30)	No discrepant events identified because observations are insufficiently detailed.	A vague statement of the difference between the prediction and the actual outcomes (e.g. "particles became bigger clumps", "saw one with 10 particles")	A clear statement of a genuine discrepancy (e.g. "we didn't predict particles forming a line")	Specific discrepant events are used as evidence to demonstrate a general discrepancy.
Evaluate reasoning based on discrepant events (Reflection #3)	No reflection is attempted.	A vague statement is made (e.g. "need to be more specific")	A specific insight is learned (e.g. "wider green part means more than two particles can be attracted to it")	A specific insight is backed up by specific evidence.

Additional Information

http://groups.mrl.uiuc.edu/granick/Publications/PDF%20files/2009/Physics_Today_Janus_Particles%20.pdf

Simulation of “Janus” Colloidal Particles

Introduction to Colloidal Particles

In this lesson, we’ll explore the behavior of colloidal particles, which are micro or nano-sized particles *suspended* in a liquid. ***Listen to your teacher describe them.***

1. What does “suspended” mean?

2. What common products have colloidal particles in them?

Brownian Motion

Here we’ll explore how colloidal particles move around.

Open the simulation by going to https://netfiles.uiuc.edu/sinkovit/www/MDApplet.html. ***Leave all of the settings unchanged, for now, and reduce the number of particles to 1. Start the simulation. Observe the motion of the particle. You can reduce the animation speed to see the motion slowed down.***

3. Describe the motion of the particle.

4. Colloidal particles really move like this. Why do you think the particles move this way? (Hint: think of how the particles are suspended.)

Phases of Matter

Here we’ll see how temperature changes the structure of particles that are attractive.

Add particles to get 200 in the system. Make sure the particles are all green (Janus Balance=180) and the thermostat is set to 1.00.

5. Based on the collective motion of the particles, what phase of matter (solid, liquid, gas) would best describe them? Why?

Reduce the temperature by turning down the thermostat gradually by clicking on the left arrow until you see a change in behavior. When you see the change, stop.

6. What change did you see?

7. What phase of matter now best describes the particles? Why?

Continue to reduce the temperature until you see the next phase.

8. How is this phase different from the one before? What phase is this?

Heat up the sample slowly by clicking on the right arrow.
Estimate the melting point and boiling point by seeing at what temperature the system changes from one phase to another.

9. What are the melting point and boiling point?

   Melting point =

   Boiling point =

Now set the Janus balance to 0. The particles should now be all dark gray.

10. What is different about the gray particles?

11. What phase of matter are they in?

Dimers

These particles are called Janus particles because there are two sides to them. (Janus is a Greek god with two faces.) Only two green sectors attract. We'll explore the different structures that you get when you change the width of the attractive sectors of the particles.

Reduce the system to 100 particles.
Set the thermostat at 0.10. Set atom size at 20. Increase the Janus balance to 10.
Increase the timestep to about 0.030 to make things faster. Observe for a minute.

12. What happened?

13. What new structure do you see form? Draw a picture of it.

14. Two particles bonded together are called *dimers*.
    Pause the system and count how many dimers you see. This is your ***reference state***.

    Number of dimers =

15. ***Varying temperature: Increase the thermostat to 0.15; wait a little.***

    Number of dimers =

16. What relationship do you observe between the number of dimers and temperature?

17. Provide an explanation for this relationship.

18. ***Varying the Janus balance: Return the thermostat to 0.10. Increase the Janus balance to 20.***

    Number of dimers =

19. What relationship do you observe between the number of dimers and Janus balance?

20. Provide an explanation for this relationship.

21. ***Varying the concentration: Return the Janus balance to 10. Make the system more concentrated by making the particles larger, to atoms size 30.***

    Number of dimers =

22. What relationship do you observe between concentration and the number of dimers?

23. Provide an explanation for this relationship.

Beyond Dimers

Now we'll see now increasing the width of the attractive sector of each particle will allow different structures to form.

Reset the atom size to 20, and the thermostat to 0.10 and the Janus balance to 10. Slowly increase the Janus balance up to 45 and observe carefully. Stop when you see a new structure.

24. What new structure did you observe (at around Janus balance 40 or 45)?
    Draw a picture.

25. Janus balance is a measure of the opening angle of the attractive (green) part of the particles. A Janus balance of 40, means that the attractive region extends 40 degrees to the left and right, making the attractive sector 80 degrees wide.
    Why did you not observe *trimers* at smaller Janus balances?

26. If you continued to increase the Janus balance, what structure would you expect to see next? Draw a picture. (Don't do it yet. Make a prediction!)

27. If you were to increase the Janus balance further, what other structures would you expect to see?
    Draw pictures of your predictions and write at what Janus balance you expect to see them. Make predictions of at least 3 structures. Be **specific** in your drawings.

STOP! Make sure your predictions are specific! Wait until your teacher says to go on.

Now, go ahead and continue gradually increasing the Janus balance up to 90, waiting some time in between increases. Make careful observations. Take notes below.

28. Draw pictures of the different structures you observe and the Janus balance at which you first saw them.

29. What structures appeared that you did not predict?

30. Which structures did you predict but did not observe?
    Try to explain why each these structures did not form?

31. At Janus balance 100, describe the structure you see.

32. What's another name for this? (Hint, we learned it in class yesterday.)

33. At Janus balance 130, how is the structure different?

Add a bunch more particles so that the system is quite concentrated (about 300 particles total). Let the simulation run for a little while.

34. Describe the structure that you see. Does it remind you of any common material?

35. Why are there big voids (empty spaces) in the structure?

Change the Janus balance to 180, so that the particles are completely green (attractive).

36. What happens to the voids when you do this?

37. Why does this happen? How are the non-attractive (gray) sides essential to forming voids?

Reflection Questions

1. In what ways did you observe that temperature affects structure?

2. How does the width of the attractive sector control what structures are formed?

3. How well did your predictions match your observations?
   What did you learn that will help you make better predictions in the future?