Activity Guide
Exploring Entropy

Last updated: September 1, 2023

DESCRIPTION

Your Exploring Entropy kit from Ensemble Interactives® can be used to explore many different phenomena. Below are ideas of ways to use your kit for teaching different concepts related to entropy, microscopic materials, phase changes, and energy states. This list of topics may not be exhaustive; many topics are interrelated. Check the website for the most recent compilation of suggested activities:

https://www.EnsembleInteractives.com/learning

Do you have an idea of how to use this kits or a special request? Write to us:

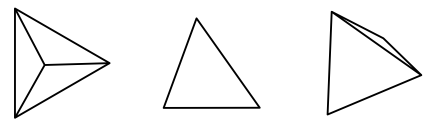
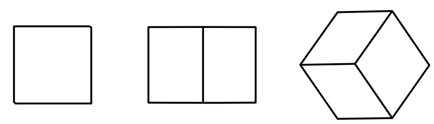
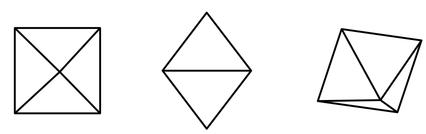
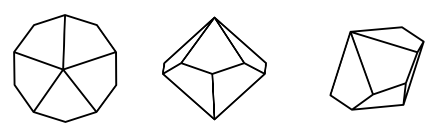
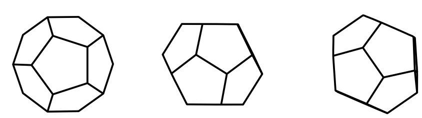
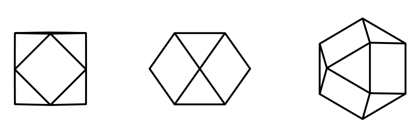
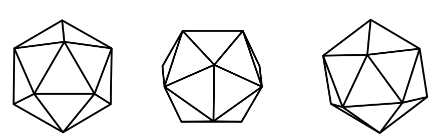
info@EnsembleInteractives.com

COMPONENTS INCLUDED

Clear plastic containers with lids	7	Tetrahedral particles	1 set
Silicone container bands	7	Cubic particles	1 set
Pouring bags	7	Octahedral particles	1 set
Corner stand	7	Pentagonal trapezohedral particles	1 set
		Dodecahedral particles	1 set
		Cuboctahedral particles	1 set
		Icosahedral particles	1 set

ENSEMBLE INTERACTIVES

Exploring Entropy particle guide

Polyhedron	Label (number of faces)	Representations
tetrahedron	d4	
cube	d6	
octahedron	d8	
pentagonal trapezohedron	d10	
dodecahedron	d12	
cuboctahedraon	d14	
icosahedron	d20	

NEXT GENERATION SCIENCE STANDARDS (NGSS)[1]

The wide range of kit activities align well with NGSS Performance Expectations (PEs) across nearly every grade level. Below is a list of PEs targeted, copied verbatim from NextGenScience.org. The associated Clarification Statements (available through the NGSS) are helpful for envisioning how to use your kit to address the PEs.

Elementary (grades K-5)	**Middle School (MS: grades 6-8)**	**High School (HS: grades 9-12)**
PS1: Matter and Interactions • 2-PS1-3. Make observations to construct an evidence-based account of how an object made of a small set of pieces can be disassembled and made into a new object. • 5-PS1-1. Develop a model to describe that matter is made of particles too small to be seen. • 5-PS1-2. Measure and graph quantities to provide evidence that regardless of the type of change that occurs when heating, cooling, or mixing substances, the total weight of matter is conserved. • 5-PS1-4. Conduct an investigation to determine whether the mixing of two or more substances results in new substances. **PS3: Energy** • 4-PS3-2. Make observations to provide evidence that energy can be transferred from place to place by sound, light, heat, and electric currents. • 4-PS3-3. Ask questions and predict outcomes about the changes in energy that occur when objects collide. **PS4: Wave Properties** • 1-PS4-1. Plan and conduct investigations to provide evidence that vibrating materials can make sound and that sound can make materials vibrate.	**PS1: Matter and Interactions** • MS-PS1-1. Develop models to describe the atomic composition of simple molecules and extended structures. • MS-PS1-2. Analyze and interpret data on the properties of substances before and after the substances interact to determine if a chemical reaction has occurred. • MS-PS1-4. Develop a model that predicts and describes changes in particle motion, temperature, and state of a pure substance when thermal energy is added or removed. **PS3: Energy** • MS-PS3-5. Construct, use, and present arguments to support the claim that when the kinetic energy of an object changes, energy is transferred to or from the object.	**PS1: Matter and Interactions** • HS-PS1-5. Apply scientific principles and evidence to provide an explanation about the effects of changing the temperature or concentration of the reacting particles on the rate at which a reaction occurs. • HS-PS1-6. Communicate scientific and technical information about why the molecular-level structure is important in the functioning of designed materials. • HS-PS1-6. Refine the design of a chemical system by specifying a change in conditions that would produce increased amounts of products at equilibrium. **PS3: Energy** • HS-PS3-1. Create a computational model to calculate the change in the energy of one component in a system when the change in energy of the other component(s) and energy flows in and out of the system are known. • HS-PS3-4. Plan and conduct an investigation to provide evidence that the transfer of thermal energy when two components of different temperature are combined within a closed system results in a more uniform energy distribution among the components in the system (second law of thermodynamics).

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SUGGESTED ACTIVITY TOPICS

- Fundamental Units as Building Blocks
- The Law of Mass Conservation
- Crystal Formation and Crystals of Multiple Elements
- Simplified Modeling of Atomic and Molecular Systems
- Reaction Rates
- Entropy and the Second Law of Thermodynamics
- Crystal Packing Patterns (SC, BCC, FCC, HCP)
- Symmetry, Symmetry Operations and Point Groups
- Computational Modeling and Numerical Simulations

ADDITIONAL MATERIALS REQUIRED

Camera or cell phone for taking pictures, ruler for measuring particle and container sizes, weighing scale, stopwatch

These materials are only required for certain activities, and are noted accordingly in the respective sections of this activity guide.

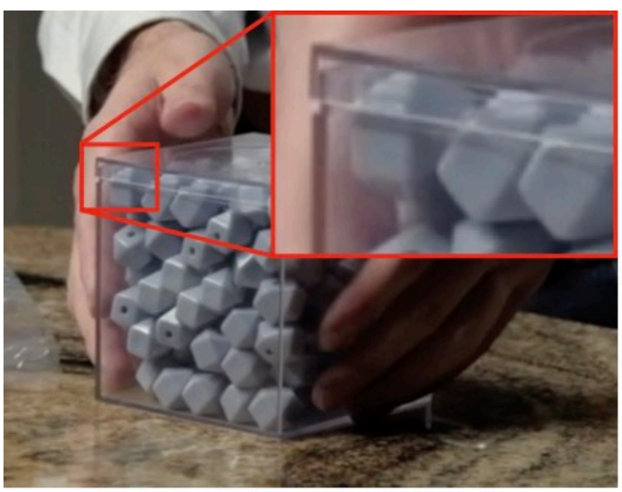
PRE-LAB ACTIVITIES

LOADING PARTICLES INTO CONTAINER

Fill the container with one of the sets of hard polyhedra. Do not attempt to stack or organize the particles in any way as you fill the container, but leave them exactly as they entered the container. Pouring the particles from a plastic bag into the container helps with this goal.




Fill the container as much as possible while still being able to fully close the lid. It is ok if you have to press moderately on the lid to get it to close or if you have to hold it closed; but the lid can not be bent or lifted in any place. If the lid can not be fully seated in its natural position, remove particles one at a time and retest the lid until it does fit.



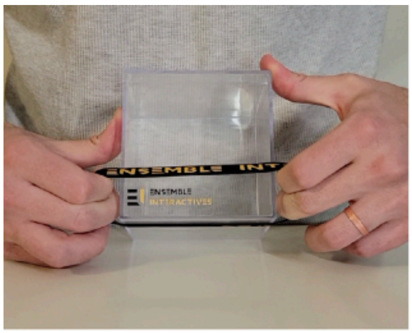
Incorrect: Lid not fully closed!

Correct: Lid closed and seated along all edges

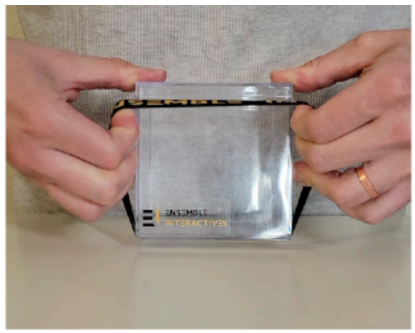
Seal the lid onto the container using the special, large silicone bands provided or a few ordinary rubber bands.

SEALING CONTAINER WITH BAND

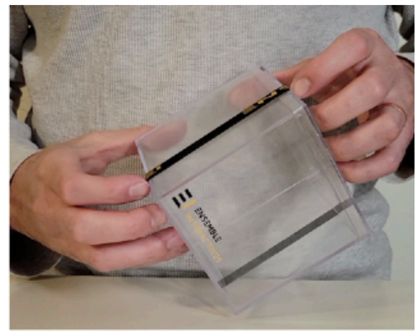
Your kit includes silicone bands used to hold the containers closed during experiments. Designed to withstand these activities' aggressive shaking, these stiff bands can be difficult to stretch over the containers. These steps are the easiest way to stretch the silicone bands:



Stretch band and hook under bottom edge of box.



Pressing thumbs on top of box, pinch thumbs and fingers together to slowly stretch band over top edge. Band is very tight!

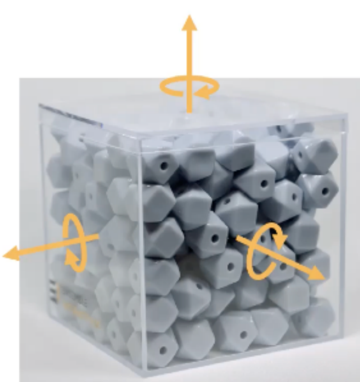


Use finger tips to slide band into center of box.

Place the band just under two bottom corners of the container, near the edge and not in the middle of the bottom face. With your thumbs pushing down on the closed lid, use both hands to stretch the band over the nearest edge of the top. Now with the band fully around the closed container, use your fingertips to pull it incrementally toward the middle.

SHAKING THE FILLED CONTAINER

Even if your container is sealed with the silicone bands included, it is still recommended to place your fingers and thumbs on opposite sides of the container to reinforce the lid while shaking, if possible. In this way, you will keep the particles from spilling out even if the band breaks.



While keeping the lid firmly sealed on the container, shake the whole system vigorously and consistently to simulate the particles having a constant temperature. Note that, in order to eliminate any appreciable effect of gravity, you must rotate the container in all directions while shaking. This can be accomplished, while shaking your hand back and forth, by turning your hand so that different sides of the container faces upward from moment to moment. Meanwhile, rotate your wrist while shaking to agitate the particles noticeably in all dimensions.

DRAWING & PHOTOGRAPHING CONFIGURATIONS

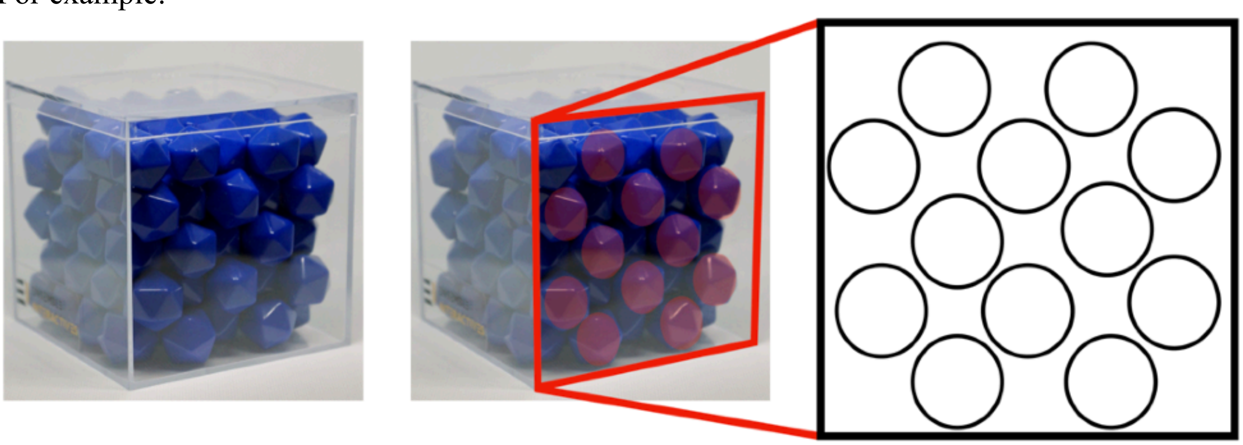
Here are some helpful tips for recording the configuration(s) of particles in a box by photographing and drawing:

When photographing, instead of moving the camera close to the box, try taking one or two steps *back away* from the box, and then zooming in with the camera. This will create a more orthographic image.

This photo was taken only 3-4 inches from the box. Notice the extreme perspective angles.

This photo was taken from over 15 inches away from the box. Notice that the true shapes are preserved.

When drawing a configuration, you can simplify the drawing by only looking at the face of the container nearest to you, and the layer of particles nearest to you within the container. In addition, the particles may be represented as some simplified shape such as circles, squares, etc. For example:



If container looks like this...

Focus on one side only, & focus on only the particles touching the side...

Represent particles as simplified shapes to draw quicker, and sketch overall arrangement

ACTIVITIES

ELEMENTARY SCHOOL (grades K-5)

Fundamental Units as Building Blocks

Approximate target grade level: 2nd.
Aligns with NGSS: 2-PS1-3. Make observations to construct an evidence-based account of how an object made of a small set of pieces can be disassembled and made into a new object. [Examples of pieces could include blocks, building bricks, or other assorted small objects.]

BACKGROUND

The building blocks of nature are called "atoms." Builders make houses from wooden boards and bricks as building blocks. These building blocks may not look like the final house, but they are used to build the final house shape. Atoms-- nature's building blocks-- are far too small to be seen with human eyes, yet everything around us is made up of atoms. Look at any object around you: regardless of its size, shape, or color, it is made of many of these tiny atoms. Atoms can be used to build different materials, much like the same boards and bricks can be used to build many different houses.

PROCEDURE

- Take a set of uniform particles, and spread them out on a flat surface. Make sure none of the particles are stacked on top of one another.
- Allowing the particles to remain resting on the table, move two particles together until they touch as much as possible. Try combining those two particles in as many different ways as you can without lifting them off the table.
- Now combine several particles by making them all touch as much as possible. Without stacking them, try to arrange them to make a single layer or "plate" of particles.
- Finally, with one solid layer on the table, try to stack more particles on top. Try to build at least three layers of particles.
- Repeat all steps with at least two different particle types.

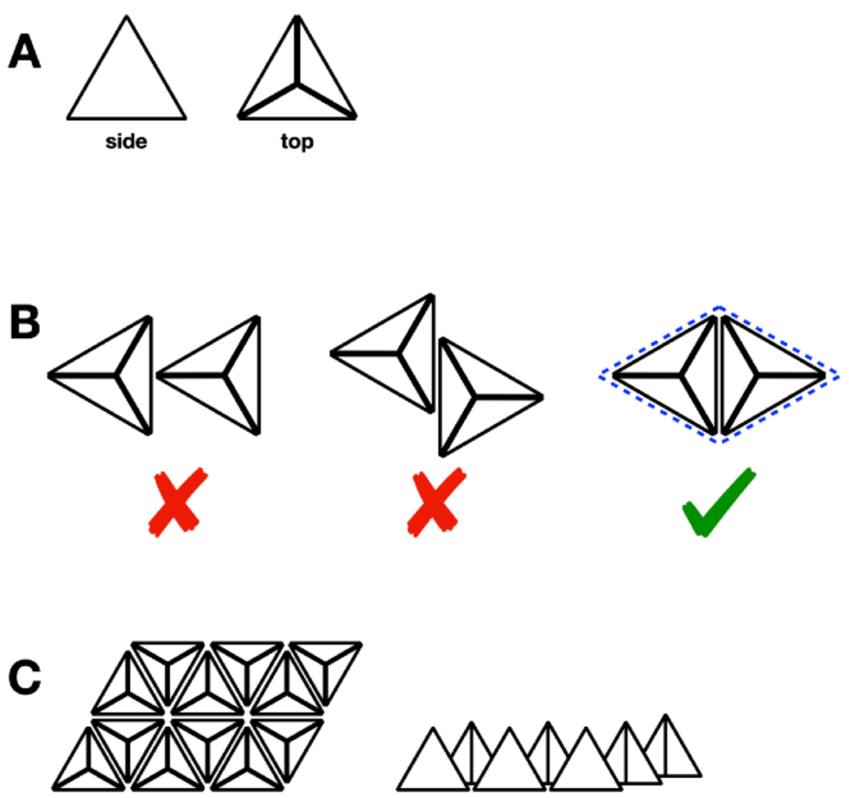
ANALYSIS

For each type of particle tested, consider the following:

- What is the overall shape of one single particle?
- When two particles are put together, what is their overall shape? Is it different from one particle alone?
- How many different ways can two particles be combined to make a new shape?
- Can several particles be combined in different ways to make a layer? What is the overall shape of the (2D) layer? Is it different from the individual particles? Is it different from two particles put together?
- Can multiple layers of particles be combined in different ways to build a structure? What is the overall shape of the (3D) structure? Is it different from the individual particles? Is it different from two particles put together? Is it different from the shape of the (2D) layer?

TEACHERS' NOTES & ACTIVITY EXTENSIONS

Considering the case of the tetrahedron (d4) particles, refer to this figure to understand each step of the ANALYSIS section:



Panel A shows how the tetrahedron is depicted in these drawings from both a top and side view. If allowed to look from one side only, students may note that it is a "triangle;" although in three dimensions, one should call it a "pyramid" or (most properly) a "tetrahedron."

Panel B shows how two particles are to be assembled "until they touch as much as possible" into an overall shape. The overall shape of this combined unit should be noted as a "rhombus," depicted by the blue, dotted line.

Panel C shows top and side views of several several particles combined (all touching as much as possible) into a 2D layer. The overall shape of the 2D layer in this example would be a parallelogram; though other perimeter shapes could also be created from a 2D layer of tetrahedra.

When stacking particles to create multiple layers, it may be helpful to build the first 2D layer inside the container (without lid), or use the lid upside down as a small tray to help contain the particles. There may be several ways the particles can stack (stably) into a 3D structure.

The Law of Mass Conservation

Approximate target grade level: 5th.
Aligns with NGSS: 5-PS1-2. Measure and graph quantities to provide evidence that regardless of the type of change that occurs when heating, cooling, or mixing substances, the total weight of matter is conserved. [Examples of reactions or changes could include phase changes, dissolving, and mixing that form new substances.] [Assessment Boundary: Assessment does not include distinguishing mass and weight.]

MATERIALS

Scale for weighing, corner stand for cubic container; OPTIONAL: camera

BACKGROUND

The Law of Conservation of Mass states that "Matter is neither created nor destroyed," even though it may change its form or appearance. Some examples of matter changing form or appearance include:

- Sugar crystals dissolving in a glass of water
- Hard spaghetti noodles in boiling water becoming soft and flexible
- Ice melting
- Melted wax turning into a solid candle.

In each of these examples, the natural materials may change their color, shape, or size. But the Law of Conservation of Mass tells us that the same amount of material exists before and after the change.

PROCEDURE

- Place a clear box in the stand so that it balances on its corner, with the open side facing you.
- Create a block in the cube by stacking particles on one another by hand. Stop building once the container is approximately half full, and place the lid on the container.
- Carefully transfer this system to a scale, and weigh the structure you built along with the container. During this process, make sure not to disturb the shape of your structure.
- Record the shape of the structure you built, either with a drawing or a photo.
- With the lid held securely in place, shake the container for five seconds.
- Record the new shape of the particles in the box, either with a drawing or a photo.
- Without reorganizing the particles, return the box to the scale to measure the final weight.
- Repeat all steps with at least one more type of particles.

ANALYSIS

- Complete the table below for the particles you tested:

Unit particle	Initial overall shape	Initial weight	Final overall shape	Final weight

- Can you think of a process in real life when matter changes, for which this system could be a model?
- What happened when you shook the container after you carefully built a structure?
- Did the weight change before and after shaking the container?
- Based on your experiments, can you explain the Law of Conservation of Mass? Is it true? Why or why not?

TEACHERS' NOTES & ACTIVITY EXTENSIONS

Students should identify that the system transforms from initially dense and ordered to a more random (and often less dense) arrangement. Thus, "melting," "evaporation," or "sublimation" may be acceptable answers for a real process being modeled.

Crystal Formation and Crystals of Multiple Elements

Approximate target grade level: 5th.
Aligns with NGSS: 5-PS1-4. Conduct an investigation to determine whether the mixing of two or more substances results in new substances. [N/A]

BACKGROUND

Many common substances such as sugar, clear diamonds, and some metals are made up of one element or only one type of molecule. These are called pure substances. However, many useful substances can also be created by mixing two or more types of atoms or molecules together. Examples of mixed substances include table salt, colored gemstones, and certain metals known as "alloys."

PROCEDURE

- Fill the container with one type of particle. Shake the container to create the "crystal" structure with that particle type.
- Record (draw or photograph) the way the particles are arranged after they have been shaken.
- Now, put approximately half of the particles back in the pouring bag, and replace the other half with a different particle type. Tumble the bag to mix the particles.
- Fill the container with the mixture of two types of particles. Shake the container with the lid sealed to create a new structure.
- Repeat all steps with a few different types of particles.

ANALYSIS

- Complete the table below for the particles you tested:

Unit particle(s)	Overall structure	Unit particle(s)	Overall structure

- How do the structures resulting from one type of particle compare to the structures you observed when two types of particles were combined? Are there any differences you can spot in the overall shape? What about in the patterns of how the particles line up?

TEACHERS' NOTES & ACTIVITY EXTENSIONS

The formation of a regular, crystal-like structure in these containers requires a fairly high density of particles; i.e. make sure students fill the containers quite full, as in the prelab tutorial videos.

The suggested grade school learning objectives are focused on recognizing patterns and/or repeating units in extended arrays of particles rather than naming specific crystal packing structures. Students should note that different particles lead to different "crystal" patterns, but may not be expected to characterize the patterns at any deeper level of complexity.

MIDDLE SCHOOL (grades 6-8)

Simplified Modeling of Atomic and Molecular Systems

Approximate target grade level: 6th-8th.
Aligns with NGSS: MS-PS1-1. Develop models to describe the atomic composition of simple molecules and extended structures. [Emphasis is on developing models of molecules that vary in complexity. Examples of simple molecules could include ammonia and methanol. Examples of extended structures could include sodium chloride or diamonds. Examples of molecular-level models could include drawings, 3D ball and stick structures, or computer representations showing different molecules with different types of atoms.] [Assessment Boundary: Assessment does not include valence electrons and bonding energy, discussing the ionic nature of subunits of complex structures, or a complete depiction of all individual atoms in a complex molecule or extended structure.]

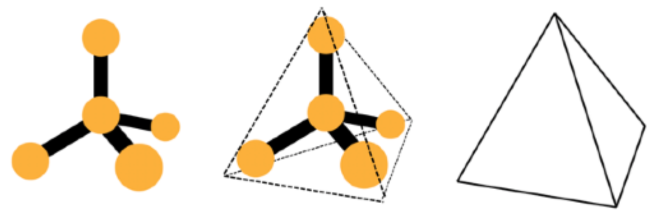
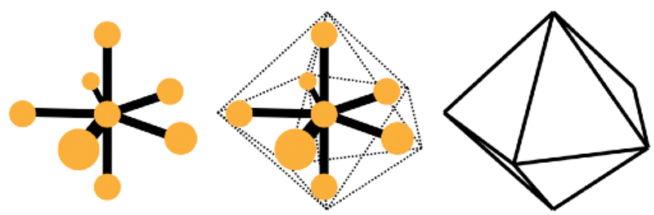
BACKGROUND

Models are used throughout science to simplify complex subjects, and help researchers understand certain aspects of a topic, even if the full topic is too difficult to understand all at once. By "model," we mean a partially-accurate representation of some real object or phenomenon. The model is valuable because it can accurately reflect some key properties, even though it is not perfect in all regards. For example, both paper airplanes and die-cast toy airplanes are models of real airplanes: the paper airplane models flight but not the shape of a true airplane, while the die-cast toy accurately models the shape but can not fly.

Scientists use simplified models of atoms and molecules. Because molecules are too small to see with human eyes and can have complex interactions, even state-of-the-art researchers often utilize "hard particle" models. Hard particle models treat atoms and molecules as polygons that can bounce off or stack upon each other, but can not be squished or broken.

PROCEDURE & ANALYSIS 1

- Choose one type of particle, and find corresponding molecule from the list below for which that polygon could be a hard particle model.
- Place five particles in the box, and seal the lid. When this container is shaken, what phase of matter could this model?
- Fill the container approximately three-fourths full with the same particle type. When this container is shaken, what phase of matter could this model?
- Fill the container completely full with the same particle type. When this container is shaken, what phase of matter could this model?

Polygon	Representative molecule & shape classification	Molecular shape
Rods	CO_2, XeF_2, linear	
Tetrahedra	CH_4, tetrahedral NH_3, trigonal pyramidal	
Octahedra	SF_6, octahedral	
Disks	XeF_5^-, pentagonal planar	
Pentagonal trapezohedra	IF_7, pentagonal bipyramidal	

TEACHERS' NOTES & ACTIVITY EXTENSIONS 1

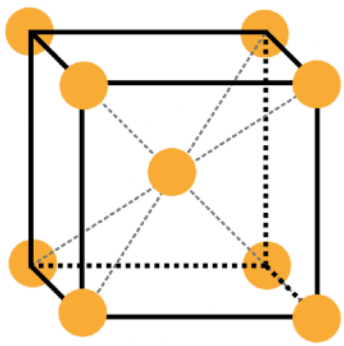
Other molecules with simple shapes such as in the table above may be available here, or from similar lists.

Only including five particles in the box is intended to model a gas, because the particles will only remain in contact momentarily. When the box is three-fourths full, it is approximating a liquid. When it is completely full, most of the available particle types will undergo an audible "phase change" while shaking, and adopt some sort of patterned structure, which is assumed to model the solid/crystalline phase.

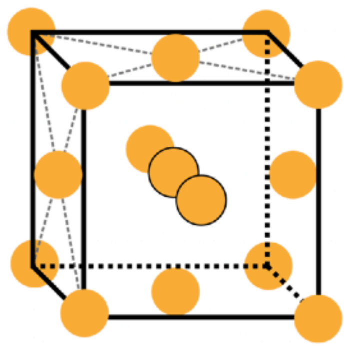
As an extension activity, students can research the actual crystal phase of their element/ molecule of choice, and evaluate whether or not their hard particle model adopts the same structure.

PROCEDURE & ANALYSIS 2

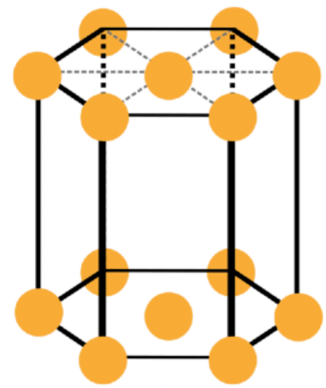
- Choose one of the metal elements from a list such as these:



Body Centered Cubic (BCC)



Face Centered Cubic (FCC)



Hexagonal

  - Table of the crystal systems (in columns) of gem minerals, with excellent photos and information for exploration on each gem: International Gem Society: Table of Gems Ordered by Crystal System
  - Periodic table listing the crystal structure of each element: Crystal structure of elements in the periodic table
- Using one or more types of particles as needed, construct a model of your element of choice according to the known structure of that element. Place the particles in the clear container manually, and create as many layers as possible/necessary to build a model of the extended crystal structure of the substance.

TEACHERS' NOTES & ACTIVITY EXTENSIONS 2

Resources: Pedagogical information about crystal packing patterns, especially SC, BCC, and FCC: LibreTexts: 8.11: Crystal Structure of Metals and 6.4: Crystal Structures of Metals

Reaction Rates

Approximate target grade level: 6th-8th.
Aligns with NGSS:

- **MS-PS1-2.** Analyze and interpret data on the properties of substances before and after the substances interact to determine if a chemical reaction has occurred. [Examples of reactions could include burning sugar or steel wool, fat reacting with sodium hydroxide, and mixing zinc with hydrogen chloride.] [Assessment Boundary: Assessment is limited to analysis of the following properties: density, melting point, boiling point, solubility, flammability, and odor.]
- **MS-PS1-4.** Develop a model that predicts and describes changes in particle motion, temperature, and state of a pure substance when thermal energy is added or removed. [Emphasis is on qualitative molecular-level models of solids, liquids, and gases to show that adding or removing thermal energy increases or decreases kinetic energy of the particles until a change of state occurs. Examples of models could include drawings and diagrams. Examples of particles could include molecules or inert atoms. Examples of pure substances could include water, carbon dioxide, and helium.]

BACKGROUND

All substances are made of either pure elements or molecules composed of the elements, or some mixture of these. Some changes a substance may undergo-- such as melting or freezing-- do not change the makeup of the substance's component atoms or molecules, but merely involve a rearrangement or phase change of those substances. On the other hand, when scientists refer to a "chemical reaction"-- such as burning or dissolving-- it is implied that some chemical bonds have been broken and/or formed, creating a new substance or substances.

PROCEDURE 1

- Using one set of polyhedral particles, fill the clear container approximately half full, and record (draw or photograph) the initial configuration of the particles.
- With the lid securely closed, shake the container for 20 seconds, or until there is an obvious audible, tactile, or visible change in the system.
- Allow the container and all particles to come to rest, and record the current configuration of the particles.
- Repeat all previous steps, adding in four particles at a time, until fewer than four particles are able to be added and the lid closed prior to shaking. Add as many particles as possible.
- After shaking the maximally full container, allowing it to come to rest, and recording its configuration, carefully remove approximately half of the particles without disturbing the configuration of any other particles.
- Finally, shake this special half-full container as described above; and record the final configuration.

ANALYSIS 1

- Complete the table below to record the configuration of the system at each stage:
- Particle type: ________________________________

Trial	Number of particles	Configuration Picture
1	approx. half full	
2	+4	
3	+8	
4	+12	
5	+16	
6	+20	
7	+_______	

- Between which two trials was the biggest change observed?
- Considering the two trials between which the biggest change was observed, can you think of a real life substance or process modeled by this experiment?
- Do you think the change observed in the containers models a chemical reaction?
- Does the change in configuration between any two trials model a chemical reaction? Why or why not?

PROCEDURE 2

- Using any number of any one particle type, arrange the particles in the container either by manual placement or random scattering. Record (draw or photograph) the initial configuration.
- With the lid securely closed, shake the container for 20 seconds, or until there is an obvious audible, tactile, or visible change in the system.
- Allow the container and all particles to come to rest, and record the final configuration of the particles.
- Repeat these steps with two other particle types. You may choose a different number and arrangement of particles each time.

ANALYSIS 2

- Considering each trial, can you think of a real life substance or process modeled by those particles and/or initial configuration?
- Do you think the change observed in the containers models a chemical reaction? Why or why not?

PROCEDURE 3

- Construct a model substance by manually stacking particles in the container, building at least three layers of particles, but also leaving the container approximately half empty.
- Keeping the bottom of the container resting on a table and the lid firmly closed, shake the container gently back and forth, slowing increasing the speed of shaking.
- Watch and listen to the container as you shake it, continuing until the model you initially built has been completely destroyed. (That is, if you pause shaking, you should no longer be able to identify the model initially constructed.)

ANALYSIS 3

- Which of the three phases of substance was modeled by the initial stack of particles?
- Which of the three phases of substance was modeled by the final configuration of the particles?
- What happened to the energy of the system throughout the process? (Hint: describe the initial energy state of the system, and any changes you effected.)
- Were there any changes in the kinetic of the particles? If so, how were these changes related to the phase of the system throughout the process?

TEACHERS' NOTES & ACTIVITY EXTENSIONS

By leaving most particles out of the kit, the low density approximates a liquid or gas system. When the system is shaken (simulating temperature via particle motion), the particles will rearrange, but always in a "disorderly" arrangement-- much like a fluid. Then, as the density is increased by adding more particles are added to the container, shaking at the same "temperature" will eventually induce a spontaneous "freezing" or "crystallization" of the system. This helps demonstrate the effects of increasing pressure on common systems, often leading toward solid phases in a phase diagram.

HIGH SCHOOL (grades 9-12)

Reaction Rates

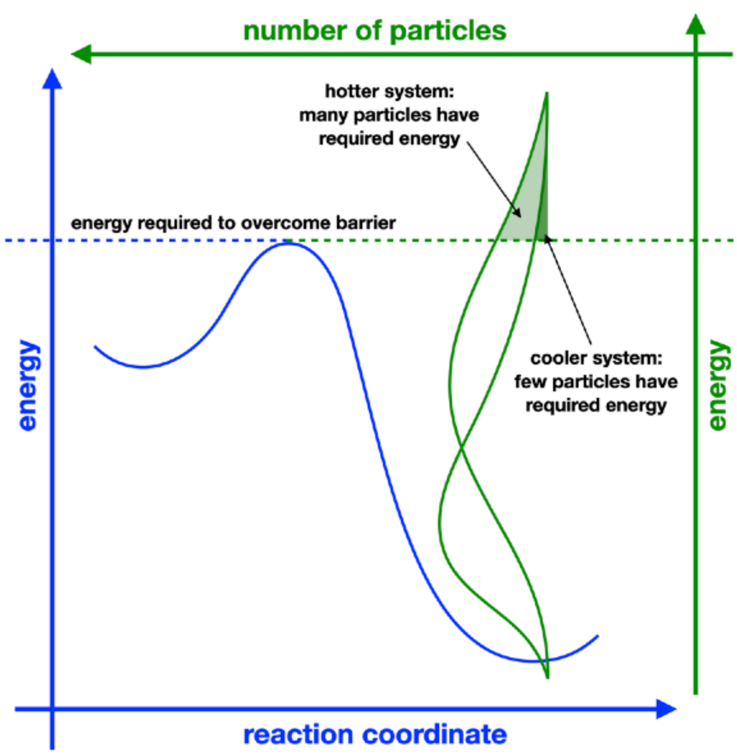
Approximate target grade level: 9th-12th.
Aligns with NGSS: HS-PS1-5. Apply scientific principles and evidence to provide an explanation about the effects of changing the temperature or concentration of the reacting particles on the rate at which a reaction occurs. [Emphasis is on student reasoning that focuses on the number and energy of collisions between molecules.] [Assessment Boundary: Assessment is limited to simple reactions in which there are only two reactants; evidence from temperature, concentration, and rate data; and qualitative relationships between rate and temperature.]

MATERIALS

Stopwatch

BACKGROUND

Under ordinary circumstances, a chemical system's temperature affects the *rate* at which some process occurs, but not *which* process occurs. Some naturally occurring processes that take a very long time can be hastened by increasing the system temperature. For example, consider a simple system that we wish to overcome a small energy barrier and relax to a low-energy state. When the system has a high temperature, there are many particles at any point in time that have sufficient energy to overcome the barrier and move to the low-energy state; thus the process happens quickly. Even when the system is cooler, *there are still some* particles that have enough energy to make the transition; just not as many at any point in time, and so the process is slower.



Since high density favors the solid phase, a disordered liquid phase will transition into an ordered solid phase when compressed with sufficient pressure and allowed sufficient time. In this activity, you will experiment with a model of such a liquid at high density; and observe the effect of the temperature on the rate of the phase transition process.

PROCEDURE

- Fill the container with any single type of particle, making sure the lid can still be fully closed and sealed with a band. Notice the initially disordered configuration of the particles, which models a liquid state of matter.
- You will provide the system energy by shaking the filled container. Soft shaking provides only a little energy, while vigorous shaking provides more energy.
- Once the system is fully prepared, start recording time on the stopwatch, and begin shaking the container.
- Shake the container gently, and try to produce a constant "temperature" by using a constant shaking speed.
- Continue shaking until an obvious change in the particle rattling sound is heard, which usually indicates the "phase change" in the particles. Pause the stopwatch when this change is heard, and check for the solid state of matter, indicated by a regular, crystal-like pattern of the particles. If the particles have a patterned configuration, note the length of time required for this phase change. If the particles still represent a liquid phase, unpause the stopwatch and resume shaking.
- Continue shaking until the phase change has been observed or 120 seconds have passed, whichever comes first.
- Repeat all steps with a medium shaking speed, and then again with a high shaking speed. In all three trials, make sure to record the length of time required to produce the phase change.

ANALYSIS

- At which shaking "temperature"-- low, medium, or high-- did the system undergo the phase change the fastest?
- Describe the kinetic energy of the particles throughout the system while it was being shaken.
- Considering the kinetic energy of individual particles, can you explain why one trial produced the phase change more rapidly?
- Construct a general, qualitative statement about why increasing temperature increases the rate of a chemical reaction or process.

TEACHERS' NOTES & ACTIVITY EXTENSIONS

Associated reading: LibreTexts: The Effect of Temperature on Reaction Rates

This discussion focuses on the use of the word "process" instead of "reaction," because "reaction" implies an exchange of atoms and/or electrons, whereas "process" is a more general term that can include non-reaction phenomena such as melting/freezing, balls rolling down hills, etc.

Students may be confused as to why a higher "temperature" favors the creation of the "solid" phase in this experiment; whereas common experience shows that solids are created by removing energy and freezing. To explain this, it is simple enough to note that if you placed a ball *with zero energy* in the left "well" of the reaction coordinate diagram above, it could not move at all. It *must* have *some* energy to overcome the barrier. Once it crosses over the barrier and "rolls down the hill," removing its energy would *keep* it at the bottom of the hill. But if it truly had *no energy* initially, it could never make the climb over the hill!

Furthermore, if we imagine repeatedly kicking the ball, one kick might send it down the hill while the next might send it back up the hill! In the case of freezing water, the molecules remain frozen as long as they are kept at low energy *once they reach the frozen state*. One should also keep in mind that it only takes a very tiny amount of energy to rotate or bend a molecule--which is the sort of "process" required to align the molecules into their solid formation. The reaction coordinate diagram above is not to-scale if one is considering the minuscule (but real) energy barrier that would be present for liquid water molecules to transition into a solid formation.

Interestingly, a challenge question for students could be to use this experiment to develop an explanation for the so-called Mpemba effect. (But see also this refutation.)

Entropy and the Second Law of Thermodynamics

Approximate target grade level: 9th-12th, college freshmen
Aligns with NGSS: HS-PS3-4. Plan and conduct an investigation to provide evidence that the transfer of thermal energy when two components of different temperature are combined within a closed system results in a more uniform energy distribution among the components in the system (second law of thermodynamics). [Emphasis is on analyzing data from student investigations and using mathematical thinking to describe the energy changes both quantitatively and conceptually. Examples of investigations could include mixing liquids at different initial temperatures or adding objects at different temperatures to water.] [Assessment Boundary: Assessment is limited to investigations based on materials and tools provided to students.]

BACKGROUND

The second law of thermodynamics states that the entropy change in the universe during any process will either increase or remain the same. Mathematically, this law is represented by:

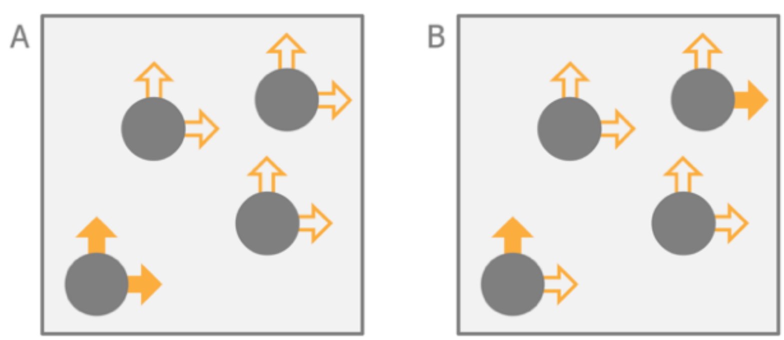
$$\Delta S_{universe} \geq 0.$$

Sometimes this law is incorrectly stated as "the disorder in the universe is always increasing." But this is incorrect, because the word "entropy" does not carry any implication about order or disorder. While it is often true that increases in entropy are correlated to increases in disorder, no physical law guarantees such a correlation, and sometimes they aren't correlated. Simply put, *entropy is the number of ways the energy could be arranged within a system.*

In order to understand entropy according to the definition above, we will need to keep track of the number of energy units belonging to the system. Within the system, each unit of energy resides in some mode of kinetic motion (such as a particle's ability to translate or rotate) or potential energy storage (such as a spring between two objects or a chemical bond between two atoms). These are the only types of places energy can exist— in either kinetic or potential energy modes. In a very simple system in which the potential energy could be ignored, all the energy would have to exist in the form of kinetic energy in the system's particles.

In the definition of entropy, "the number of ways the energy could be arranged" refers to all possible ways of distributing the system's units of energy among the particles. Figure 3 shows two different criteria for distributing two units of energy throughout a simple system. When there are more possible ways the energy is allowed to be arranged among the energetic modes, the entropy is greater.

Consider this figure, showing a very simple 2D system, composed of four particles but possessing only two units of energy. In image A, one particle possesses both units of energy, which can only happen 4 ways. In image B, however the units of energy are spread across 2 particles. In this case, there are 24 unique arrangements of the energy units possible! If a system such as that shown in the figure transitioned from state A to state B, $\Delta S > 0$, because $S_B > S_A$, meaning an increase in entropy.



Derivation of the model.

The model system we will use in this lab includes a collection of hard, polyhedral particles to simulate atoms or molecules and a rigid container to ensure a constant volume. By shaking the container, we will simulate the constant random motion of real particles. The thermodynamic conditions in this system are special because they allow us to confidently conclude that any visible changes in the system are a direct result of changes in the system's entropy. The remainder of this section shows how this conclusion is derived.

You should have already learned elsewhere the definition for a change in the Gibbs free energy:

$$\Delta G = \Delta H - T\Delta S \qquad \text{(Eq.1)}$$

in which T is the temperature (which is held constant), S is the entropy as defined above, and H is the enthalpy. If the definition of the change of enthalpy (ΔH) is applied to Eq.1, we obtain the expanded form:

$$\Delta G = \Delta U + P\Delta V - T\Delta S \qquad \text{(Eq.2)}$$

in which P is the external pressure, V is the volume, and U is the internal energy. The term "internal energy" includes the kinetic and potential energy of the system's constituents, but excludes any additional energy due to external forces (e.g. gravity, a magnetic field, etc.). It is important to note that free energy can be defined for any system and that a change in free energy can occur during any process and is not limited to chemical reactions. Therefore, Eq.2 is also applicable to the model system we will use in this procedure. Any changes in the Gibbs free energy of the model system are also governed by Eq.2.

As stated above, our model system uses a rigid container such that its volume can not change. This implies that $\Delta V = 0$ in this special case. Since the particles in our system are non-deformable and have no apparent attractions or repulsions to one another,5 the system's internal energy, U, will be defined only by the particle's kinetic energy in this special case. In addition, Eq.2 requires that the temperature, T, is constant during the process. Since a system's temperature is defined by the average kinetic energy of its particles, Eq.2 implies that there is no change in the average kinetic energy per particle during the process. Given this reasoning, Eq.2 is reduced to:

$$\Delta G = -T\Delta S \qquad \text{(Eq.3)}$$

Notice what Eq.3 implies: for any special system that obeys our assumptions, a change in free energy is just the opposite of the change in entropy, multiplied by a constant (T)! Furthermore, we know that spontaneous processes are those for which the change in free energy is less than 0:

$$\Delta G_{spontaneous} < 0 \qquad \text{(Eq.4)}$$

So, a positive ΔS, implying $S_f > S_i$, corresponds to a negative ΔG. *This is to say, if a spontaneous process occurs in the special environment outlined above, that process is guaranteed to have resulted from an increase in entropy.* This lab experiment uses a physical realization of the model system just derived to study entropy and investigate its relationship with disorder.

PROCEDURE

- Fill the container with one of the sets of hard polyhedra. Do not attempt to stack or organize the particles in any way as you fill the container, but leave them exactly as they entered the container.

- With the lid firmly in place, gently rotate the filled container in order to record (draw or photograph) this initial arrangement of the particles. This is the initial configuration or “state” of the system.
- While keeping the lid firmly sealed on the container, shake the whole system vigorously and consistently to simulate the particles having a constant temperature. Note that, in order to eliminate any appreciable effect of gravity, you must rotate the container in all directions while shaking. Shake the container for at least 10 seconds, listening for any changes in the pattern of sound.
- When you stop shaking the system, gently rotate the container to investigate this final state without disturbing the particle arrangement. Look at each face of the container for any visible patterns or organization of the particles. If you do not see any visible difference in the particles’ configuration, repeat the above steps twice more (for a total of three trials).
- After completing all necessary trials, accept the current configuration as the “final configuration.” Photograph/sketch what you see when viewing one or more faces of the container.

ANALYSIS

- As you continued to shake the system, did the sound change? If there was a noticeable change, briefly describe the change in tone, loudness, etc. If you did not notice any change in the sound, simply record “No change.”
- Describe any visible differences in the initial and final states of the physical model system.
- Can you confidently make any comparative statement(s) about the entropy of the initial and/or final states of the system?
- Can you explain your observation(s) in terms of the definition of entropy? In other words, how can your understanding of entropy be used to explain the observed process?

TEACHERS' NOTES & ACTIVITY EXTENSIONS

Derivation steps could be obscured for students to reason through these equations as analysis questions.

Crystal Packing Patterns (SC, BCC, FCC, HCP)

Approximate target grade level: 9th-12th, college freshmen

BACKGROUND

Many familiar solids are crystals, which are characterized by the periodic arrangement of their atoms to form the bulk material. Many different crystalline substances share the same periodic arrangements, despite being composed of different atoms. A few periodic arrangements-- known as "crystal packing patterns"-- characterize a very large number of crystals. While the factors that cause one element or substance to adopt a particular packing pattern are complex, the arrangements themselves can often be identified more easily. A few of the most common crystal packing patterns are known as simple cubic (SC), body-centered cubic (BCC), face-centered cubic (FCC), and hexagonal close packing (HCP).

PROCEDURE

- Fill the clear container with one type of polyhedral particle. When filled with the full set of particles provided, the particles will arrange themselves into their most efficient packing pattern when shaken.
- With the filled container firmly sealed, shake the container to allow the particles to rearrange into their preferred orientation(s).
- Continue shaking for at least 30 seconds, or until an obvious audible change indicates that the system has adopted a different configuration.

ANALYSIS

- What crystal packing pattern is adopted by each of the different polyhedra available?
- Can you recognize any of the standard packing patterns in any of the "crystallized" polyhedral systems?
- Complete the table below.
- Manually construct a system according to two of the known packing patterns.

Polyhedra (dN)	Approximate packing pattern	Drawing or photo of representative configuration

TEACHERS' NOTES & ACTIVITY EXTENSIONS

When filled with the full set of particles provided, the dense systems will spontaneously self-arrange into common packing structures such as simple cubic (SC), face-centered cubic (FCC), hexagonal close packing (HCP), or body-centered cubic (BCC). Certain polyhedra with particularly interesting dense packing structures are as follows:

Shape	Approximate packing structure
d4	complex
d6	SC
d8	SC, with additional particle alignments; interstitial defect possible
d10	unapparent
d12	complex
d14	SC
d20	BCC or FCC or HCP

Resources: Pedagogical information about crystal packing patterns, especially SC, BCC, and FCC: LibreTexts: 8.11: Crystal Structure of Metals and 6.4: Crystal Structures of Metals

Symmetry, Symmetry Operations and Point Groups

Approximate target grade level: 12th, college

BACKGROUND

The famous physicist Richard Feynman described "symmetry" by noting, "Professor Hermann Weyl has given this definition of symmetry: a thing is symmetrical if one can subject it to a certain operation and it appears exactly the same after the operation... a thing is symmetrical if there is something we can do to it so that after we have done it, it looks the same as it did before."[2] Mathematics has produced a set of symmetry "point groups," which are essentially labels to describe all the types of symmetry an object possesses. In chemistry, understanding the symmetry point group of an atom or molecule can give rapid insights into the shape of its electron's orbitals, predicting what types of interactions and bonds can be made with other molecules. For these reasons, students practice identifying the point groups of simple objects to become familiar with the properties of different symmetry elements.

Some specific symmetry elements relevant to the shapes provided are a "symmetry plane," "inversion center," "proper axis," and "improper axis."

PROCEDURE

- Follow the tutorial (https://symotter.org/tutorial/intro) to learn about different symmetry elements/operations.
- For each type of polyhedral particle, identify as many symmetry elements as you can.
- For one particle at a time, follow the flow chart (https://symotter.org/assets/flowchart.pdf) to identify the particle's point group.

ANALYSIS

- Fill in the table below with the symmetry element(s) and point group(s) you identified for each particle.

Polyhedron	Symmetry Elements	Point Group

- Find the polyhedra you studied in the interactive gallery (https://symotter.org/gallery). Are the symmetry elements you identified correct? Are there any additional elements you missed?

[2] Feynman, Richard P. Six Easy Pieces and Six Not-so-Easy Pieces: Essentials of Physics Explained by Its Most Brilliant Teacher. Perseus Books, 2001., chapters 1, 2

TEACHERS' NOTES & ACTIVITY EXTENSIONS

The full lab kit includes various polyhedra (d4, d6, d8, d10, d12, d14, d20) with different symmetries, including T_d, O_h, I_h, C_{nv}. After teaching the definitions of "symmetry plane," "inversion center," "proper axis," and "improper axis," allow students to try to assign the correct point group to each polyhedron. Pairs well with online visualization tool: https://symotter.org.

Computational Modeling and Numerical Simulations

Approximate target grade level: 12th, college

BACKGROUND

Computational simulations is a quickly-growing and cutting edge area of nearly every discipline of science. Computers allow researchers to investigate many phenomena with arbitrary precision and sometimes not even experimentally accessible, testing and validating theories and making brand new discoveries. Since computers can only perform dictated programs, the accuracy of computational studies relies on the researcher's ability to translate some real phenomenon into a mathematical description. Interestingly, many seemingly-simple models can still yield valuable insights. One strategy in computational sciences is to begin with a model simple enough to be confidently programmed into a simulation, and then incrementally add complexity to the model up to the desired level of realism. Surprisingly valuable insights are often gained by approximating molecules as hard polygons.

PROCEDURE 1

Using your school's library system, find a peer-reviewed journal article describing a computational study. Specifically, find an article that uses simulations of "hard-body" polygons. Suggested journals include the following, though there are many others as well:

- Scientific Reports
- Nature
- Proceedings of the National Academy of Sciences (PNAS)
- Journal of Chemical Physics
- Journal of Physical Chemistry B
- Physical Chemistry Chemical Physics (PCCP)

You can also search for articles in many journals simultaneously by using Google Scholar.

ANALYSIS 1

While reading your article, try to identify the following:

- What process, phenomenon, or molecule is being studied?
- What question does the proposed research hope to answer?
- What polygon(s) is being used in the simulation?
- What molecule/thing is that polygon a model of?
- What shape is the simulation "container"?
- Can you construct a hands-on demo of the computational simulations using your hard-particle activity kit?
- Describe your chosen article to your classmates using your hands-on model.

TEACHERS' NOTES & ACTIVITY EXTENSIONS 1

Some appropriate journal articles can be found on the Ensemble Interactives website under the heading, "Relevant peer reviewed journal articles: Simulation & Theory References." (https://ensembleinteractives.com/learning/)

It may be easiest to find applicable articles in the chemistry and physics journals, in studies of bulk molecular systems. Such studies often involve some physical *process* rather than a chemical *reaction*.

PROCEDURE 2

You will perform a computational simulation as well as a real-life, hands-on experiment with the same hard particle system. Begin with the computational portion:

- Open up the software and load in the initial configuration of hard polygons in a box, as provided by your teacher.
- Using the computer script provided, give each of the particles a randomized initial velocity.
- Execute the simulation.

After completing the simulation, perform the same experiment with the hands-on activity kit.

ANALYSIS 2

- Check all the settings in the simulation software to make sure the simulation you are about to perform is indeed simulating the system as you wish. Can you explain what each setting controls?
- How do the initial and final configurations compare between the simulation and the hands-on kit?
- Is there any discrepancy between the real and simulated experiments? What could be done to make them more similar? (E.g. how could the simulation become more ideal or realistic? Could you invent a tool or device to make the hands-on experiment more ideal or consistent?)

TEACHERS' NOTES & ACTIVITY EXTENSIONS 2

The free, open source Blender software can be downloaded here: https://www.blender.org/download/

Advanced students can follow the in-depth tutorial to create their own initial configuration(s), which is in itself a computational simulation, and also provides some CAD experience.

If students are comfortable generating custom initial configurations, these experiments can be dramatically expanded by allowing the students to create their own polygons for testing. These polygons can also be 3D printed to allow them to carry out the hands-on portion after the numerical simulation of their custom polygon system.

CARE & MAINTENANCE

Care should be taken while securing and removing the plastic container lids, as they are prone to cracking or chipping. However, as long as the lids can still confidently index with the container body and be secured with rubber bands for the experiments, even moderately chipped lids can still serve their intended function as no fluid seal is required. For longevity of the containers, it is recommended to store as many as possible directly abutting one another, whether filled or empty. We recommend that boxes not be stored with silicone bands stretched around them, as this may lead to a gradual warping of the plastic containers.

The silicone bands for securing the container lids are very tight during normal use, and may break if stretched much more than necessary to fit around the containers. If the included bands break, other silicone or rubber bands should suffice.

The particles do not require any maintenance beyond not losing too many to still perform the activities/demonstrations. Instead of keeping a count of the hundreds of particles, we recommend checking for a sufficient number by simply filling the containers. To confidently carry out all experiments, there should be at least a few too many particles to fit within the closed containers without any special packing.

The small particles may pose a choking hazard; the plastic bags included may pose a suffocation hazard.

Replacement or additional parts can be ordered from our website. Place your specific request to us in writing: https://ensembleinteractives.com/product/spare-parts/

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