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Atomistic computational approaches in molecular models and inorganic crystallization

by

Tesia D. Janicki

A dissertation submitted in partial fulfillment of
the requirements for the degree of

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(Chemistry)

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The dissertation is approved by the following members of the Final Oral Committee:

JR Schmidt, Professor, Chemistry
Arun Yethiraj, Professor, Chemistry
Susan Babcock, Professor, Materials Science
Paul Evans, Professor, Materials Science

This cartoon is separated into two sections to highlight different areas of my PhD research.

Each section contains some background motivation before explaining my contributions.

Section I

Background

Molecular Models

My Work

Benzene Force Fields

Section II

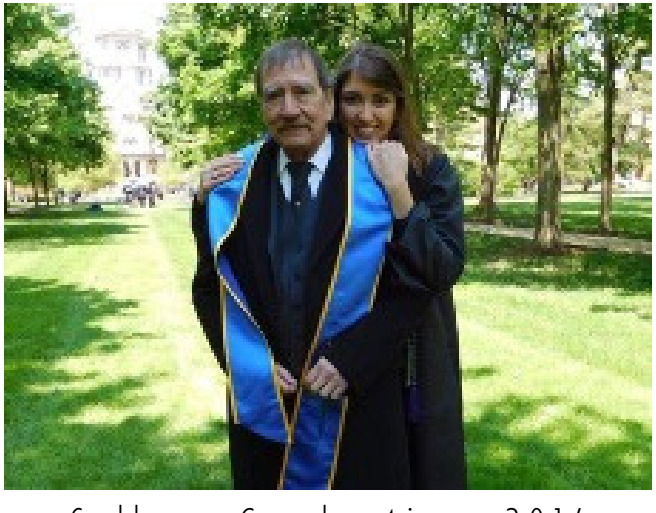
Background

Solids & Structure

My Work

Modeling Crystallization

Berry Picking, 1997



College Graduation, 2016

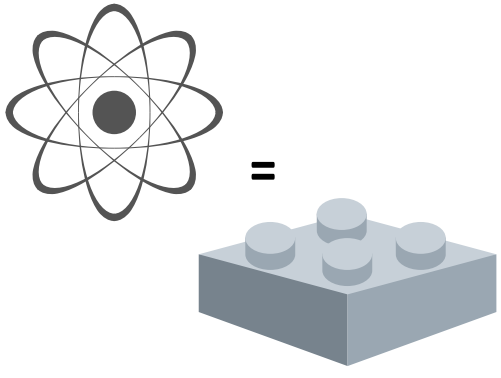
My dad inspired me to create a cartoon thesis chapter. When I first moved away from home, he would send clips from newspaper comic strips. These brought me joy during stressful exam seasons.

My dad did not have a formal college education, but he had an insatiable curiosity of the natural world. In many ways, I think of him as the first scientist I ever knew. Because of him, my childhood was filled with exploring the outdoors, stargazing, and experimenting in the kitchen.

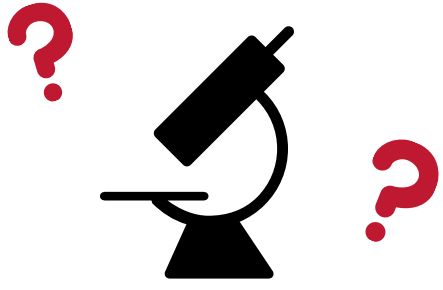
"Not knowing" is an opportunity to learn something new and exciting! I believe disseminating research in a publicly consumable format is just as essential as the research, itself. This chapter is for the scientific curiosity which lives in us all.

BACKGROUND

Molecular Models

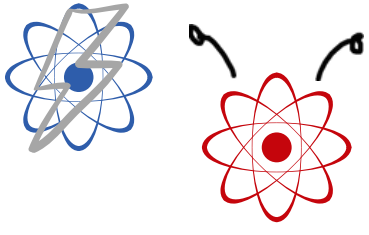


Atoms are the building blocks which make all matter in the universe.



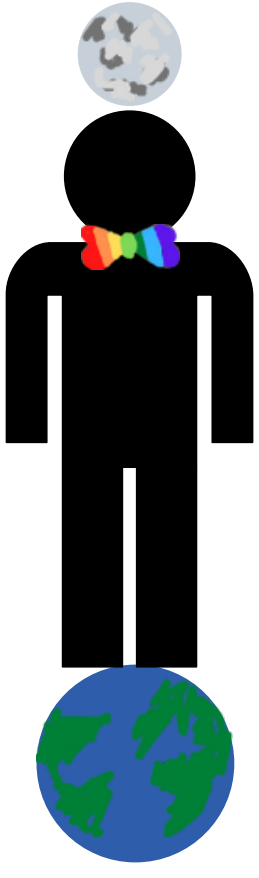
The motion of atoms is extremely hard to measure in the laboratory.

Like Quicksilver and Antman combined!



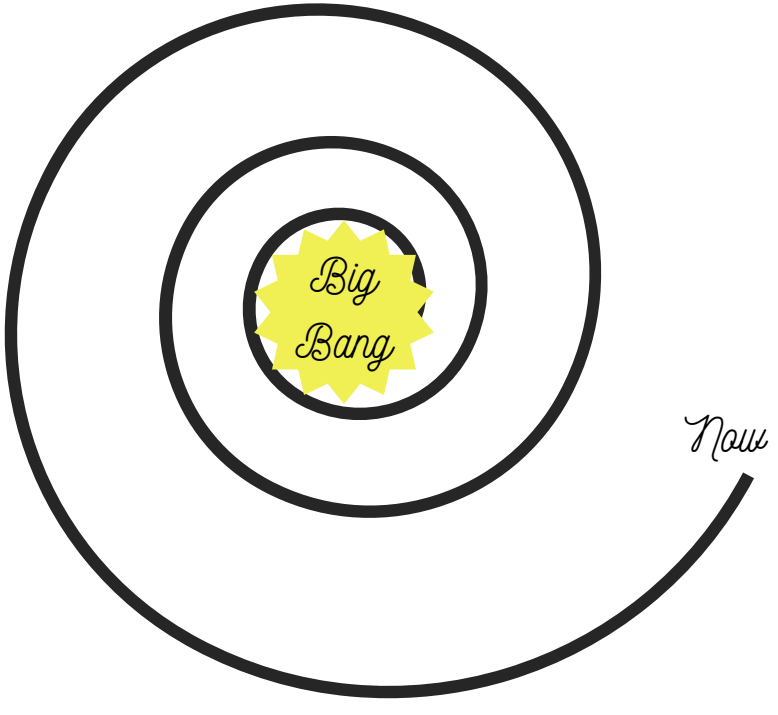
This is because atoms are very fast and very tiny.

Atoms are about 1/10,000,000,000th of a meter wide.



If an atom were the size of a marble, humans would be as tall as the distance from the earth to the moon!

Atoms move on sub-picosecond (1/1,000,000,000,000th a second!) timescales.



The difference in scale between a picosecond and a second is the same as the difference between a day and the age of the universe!

Input:
Physics!

Output:
Models!

Molecular models are used to provide estimates of atomic motion to help explain observations in the lab and the real world.

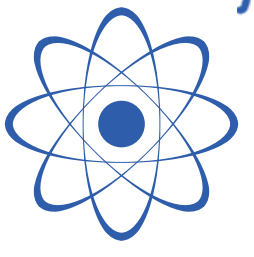
Spoiler alert!
More on this later

For example, we can use molecular models to study crystallization.

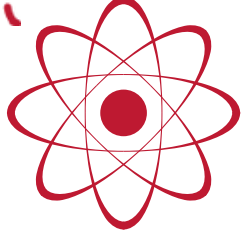
Not like Star Trek...

Force Fields are key to molecular models.

Good morning!



Nice weather today!



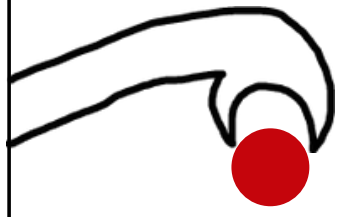
An "attractive" interaction

In chemistry, Force Fields are equations which explain how atoms interact.

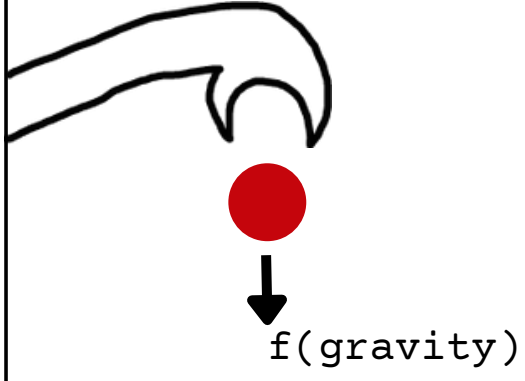
```
F = force1 +
force2 + ...
```

Force Fields are the sum of all forces present.

To explain how Force Fields work, let's use a life-size example...



Think of the motion of dropping a ball.



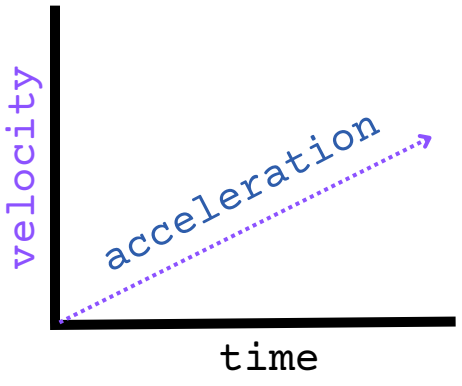
The ball drops to the ground because of a force called gravity.

```
F= f(gravity)
```

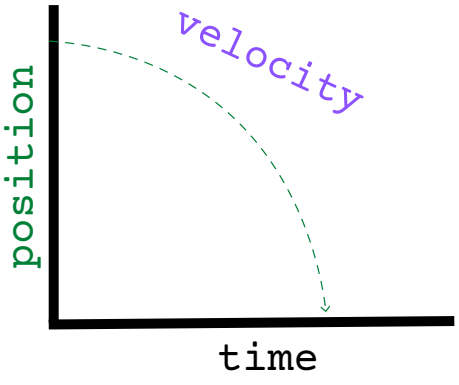
The Force Field acting on the ball includes the force of gravity.

```
F = m * a
```

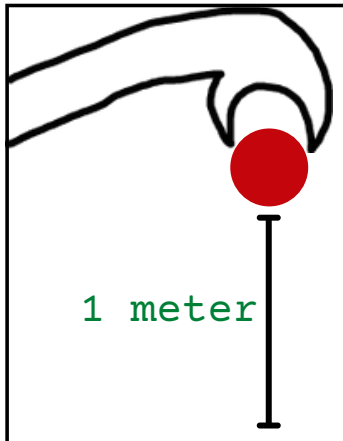
The Force Field is proportional to the mass of the ball and its acceleration.



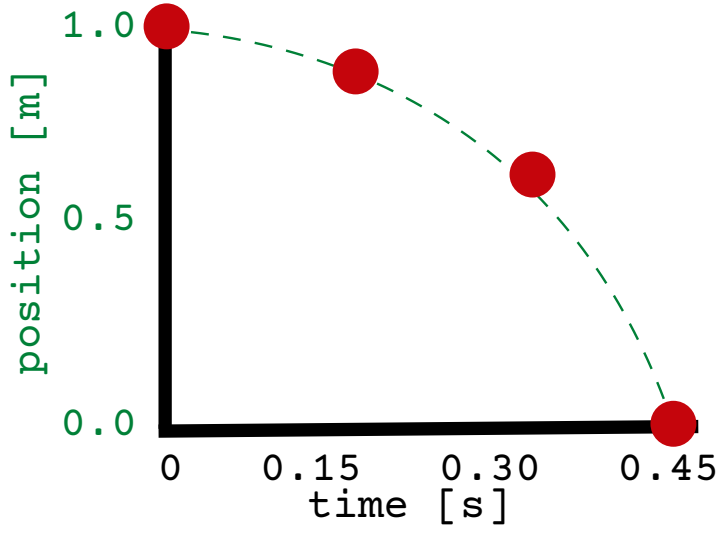
Acceleration is the rate of change of velocity.



Velocity is the rate of change of position.



If we know the initial position, mass, and the force on the ball...



We can calculate its position over time.

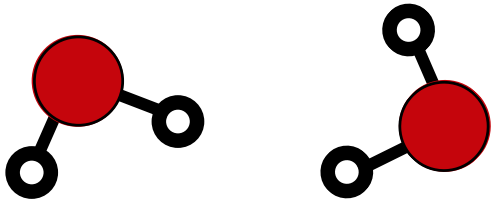
Force Fields are a little more complicated than gravity, but the same motion calculation can be applied to atoms.

Force Field development is an active area of research!

MY WORK

Benzene Force Fields

Force Fields can be simple expressions, dependent only on the distance between atoms.

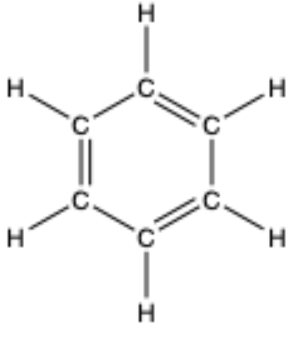


Force Fields can be more complex with additional dependence on a molecule's orientation.

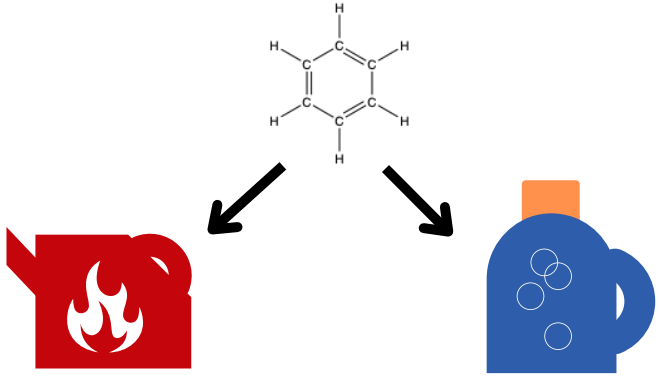
Computers are only as smart as the information we give them

In my research, I have developed software to implement Force Fields with orientational dependence.

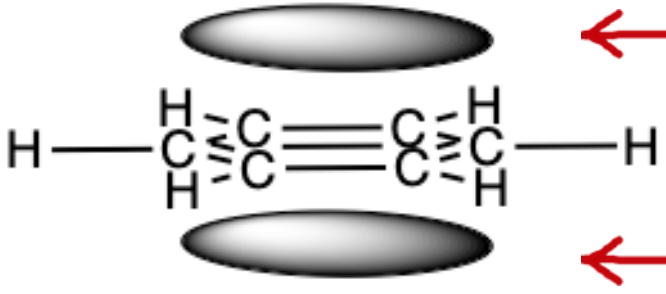
Let's see an example of how orientation could be necessary for improving accuracy...



Benzene is a molecule made of six carbon (C) and six hydrogen (H) atoms.



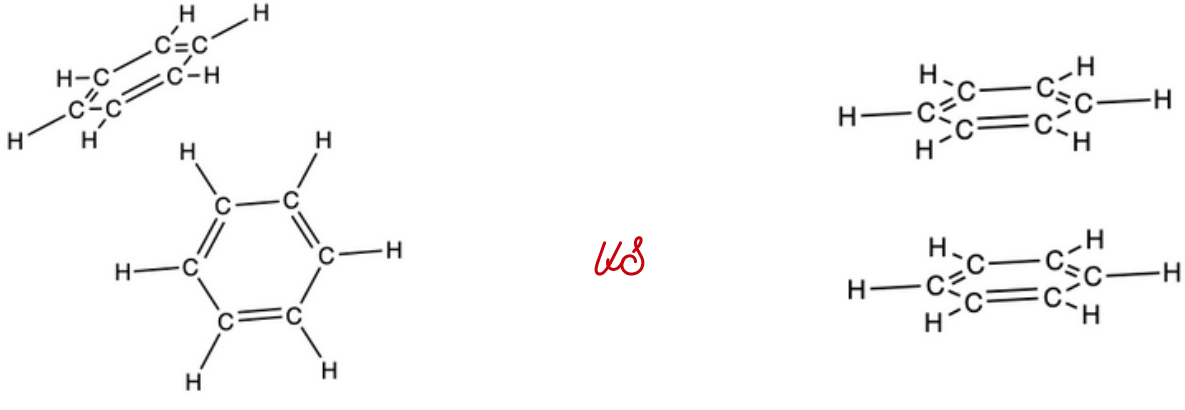
Benzene is a component of gasoline as well as some dyes and detergents. It is also poisonous!



Like two halos

Benzene is a relatively flat molecule. It has a special arrangement of electrons which exist on the top and bottom of the benzene ring.

Imagine two benzene molecules close together.

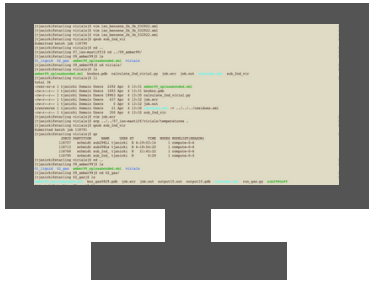


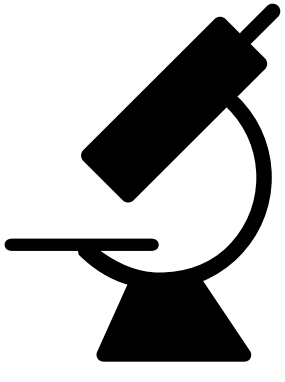
vs

The way the two molecules are arranged will impact the forces they exert on each other.

Two bar magnets behave the same way. If they are arranged like a sandwich, they will attract. If they are arranged like a "T," they will not attract.

Similar orientational dependence in benzene can be incorporated in the Force Field.

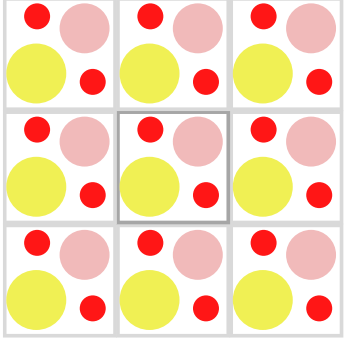




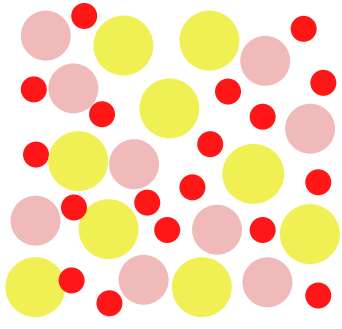
By incorporating orientational dependence, the accuracy of benzene models is improved. We can accurately reproduce "real-world" measurements!

BACKGROUND

Solids & Structure



Many solids exist as ordered crystals, which means they have a repeating unit.



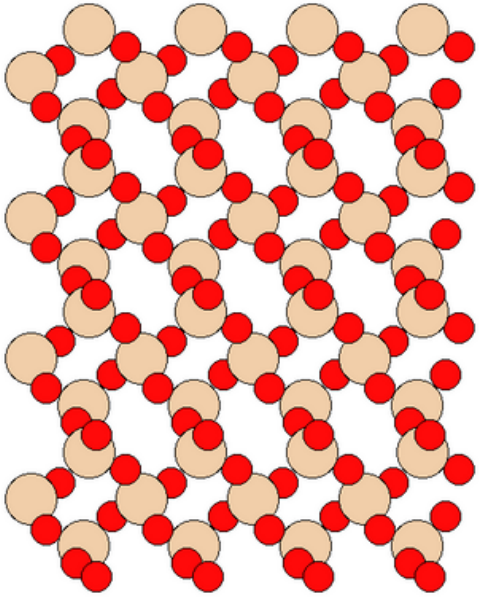
Solids can also be disordered (amorphous). There is no repeatable unit.

The same atoms can exist as either ordered crystals or amorphous solids.

Actual atomic structure of silicon dioxide as quartz*:

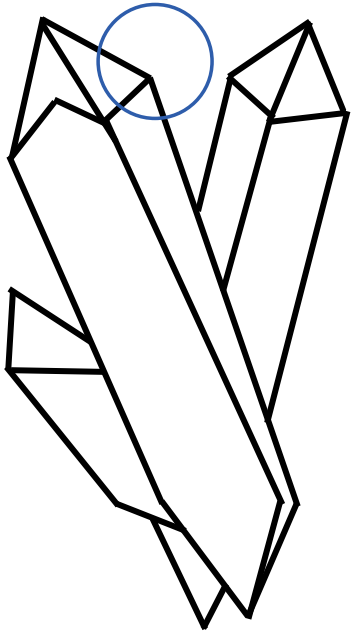
silicon

oxygen

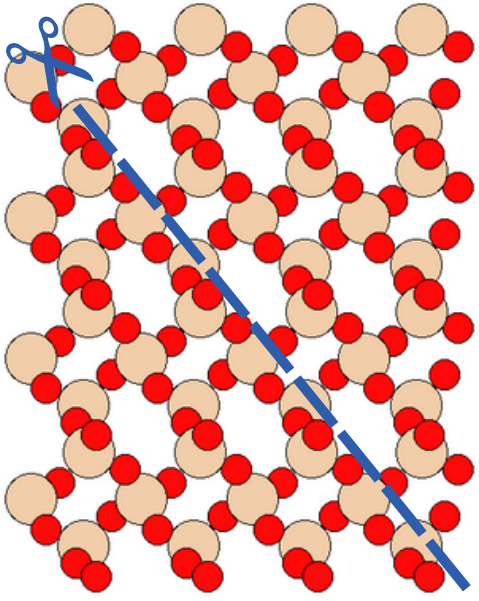


Silicon dioxide can make quartz, an ordered crystal.

Edges and angles



Atomic order dictates life-sized structure. Natural quartz shows edges.



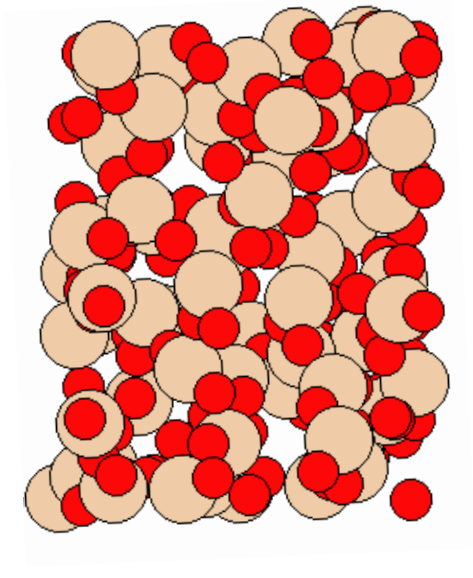
These edges occur along boundaries between layers of atoms.

*Structure from H. D'Amour, et al. *Acta Cryst.* (1979). B35, 550-555

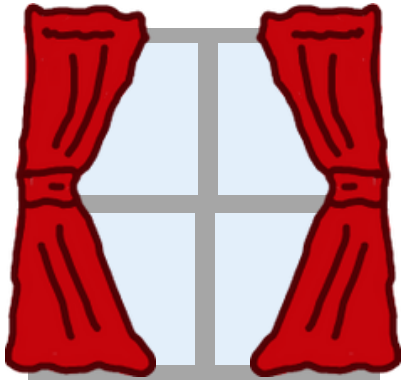
Atomic structure of amorphous silicon dioxide:

silicon

oxygen

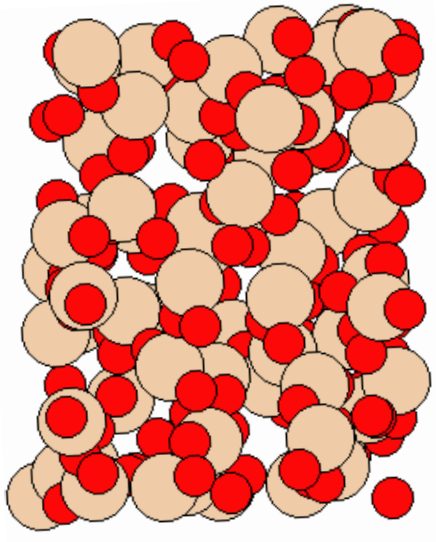


Silicon dioxide can also make glass in windows. Glass is an amorphous solid.

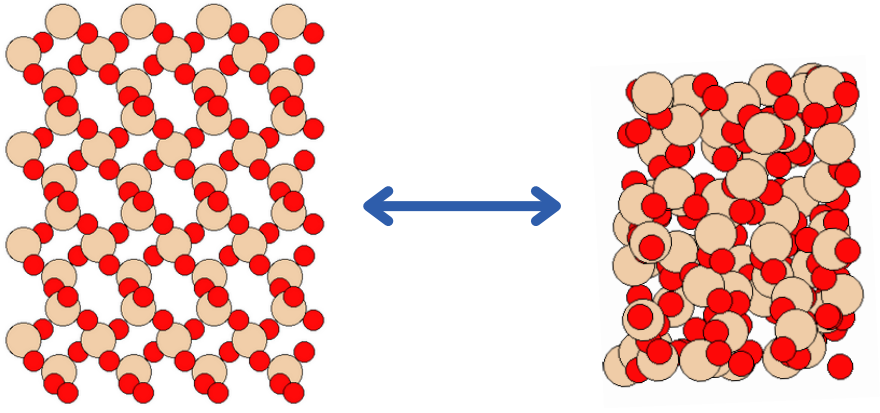


Glass appears to be smooth and can appear in many shapes.

No clear boundaries to cut between

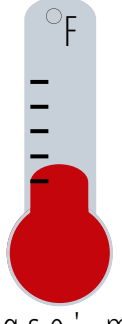


The disordered nature of the atoms do not dictate any large-scale order.

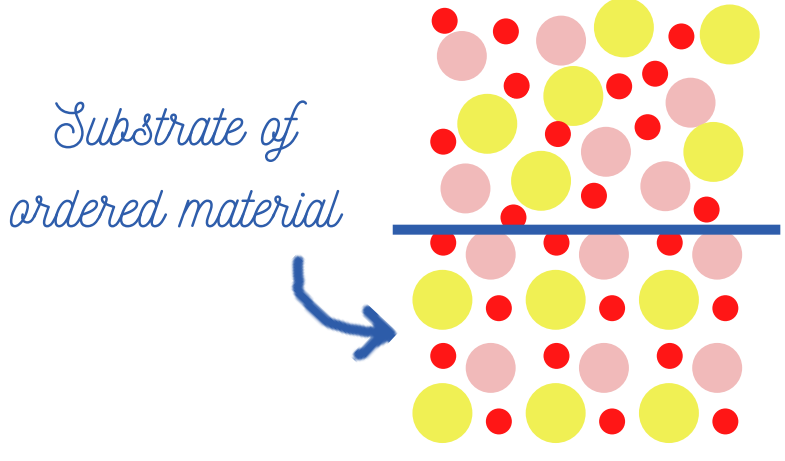


Silicon dioxide is just one of many materials which can exist as an ordered crystal or disordered solid.

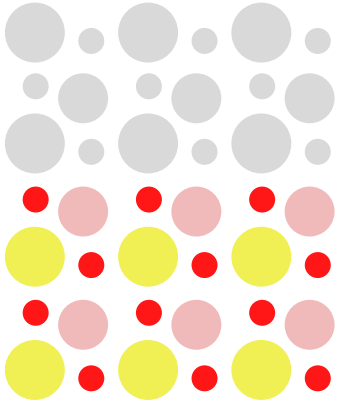
Scientists are interested in controlling how atoms arrange themselves into crystals.
One method is called solid-phase epitaxy.



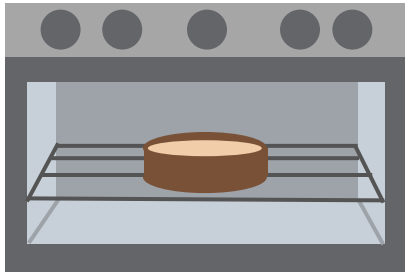
'Solid-phase' means the atoms are at low temperatures and do not flow as much like a liquid.



'Epitaxy' means crystallization occurs with guidance from a substrate - a surface template.



The substrate guides the final position of the atoms while they are heated at a low temperature.



Solid-phase epitaxy is like baking a cake: the substrate is like a cake pan, which guides the shape of the batter in the oven.

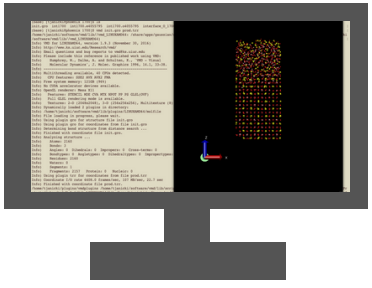
Controlling crystallization requires a precise "recipe" of experimental conditions.

Research is required to understand what conditions are required to make uniform crystals.

This can be a tricky problem and requires a lot of collaboration!

MY WORK

Modeling Crystallization



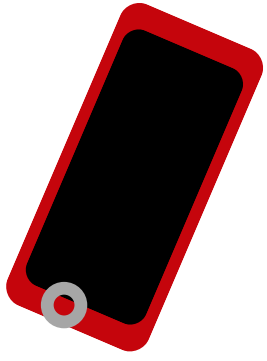
In my research, I have used models to observe atomic motion during crystallization for complex oxides.

These materials are "oxides" because they contain oxygen.

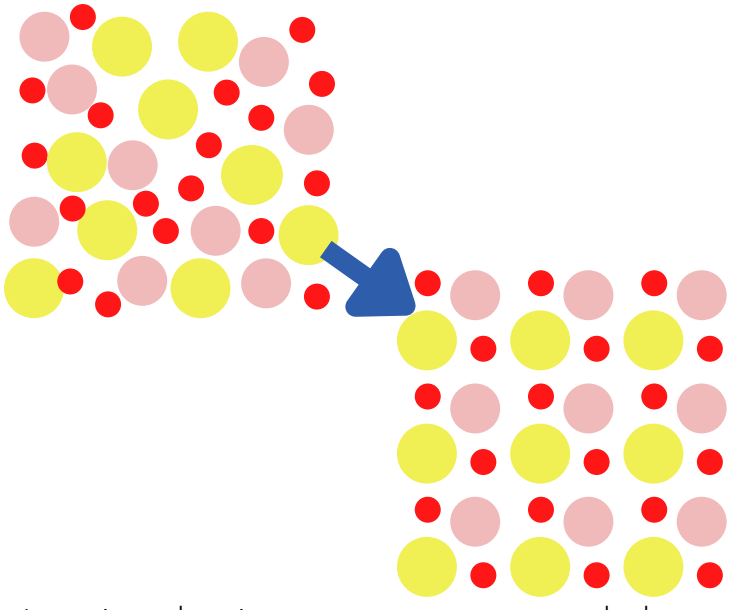
oxygen

other elements

These materials are "complex" because they contain more than one other atom type.



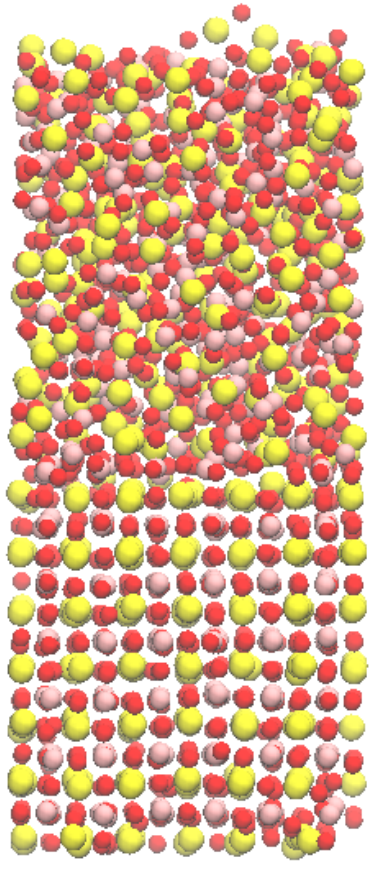
Complex oxides have applications in electronics, like your cell phone!



In simulations, we can track how atoms transition from a disordered, amorphous phase to an ordered crystal.

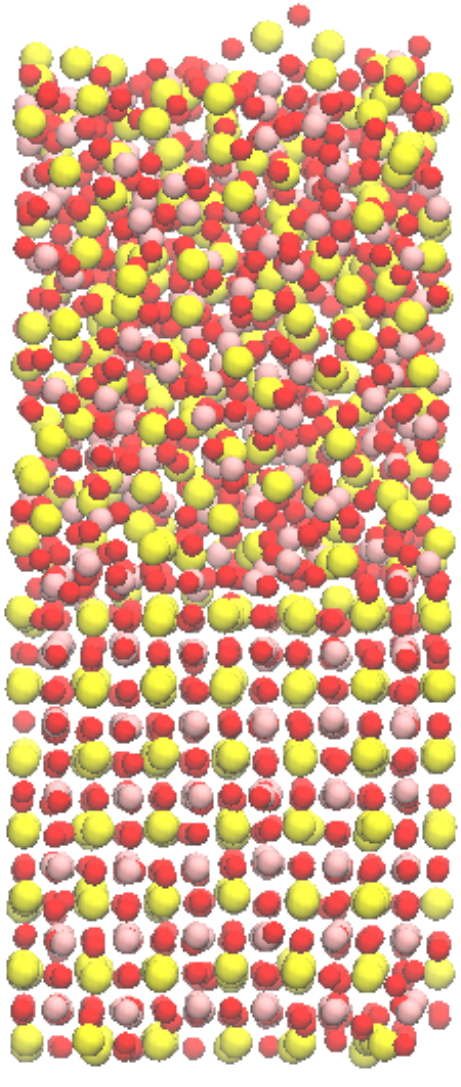
Simulations start with an initial configuration of atoms which resembles experiments.

The initial structure includes the amorphous material we want to crystallize...

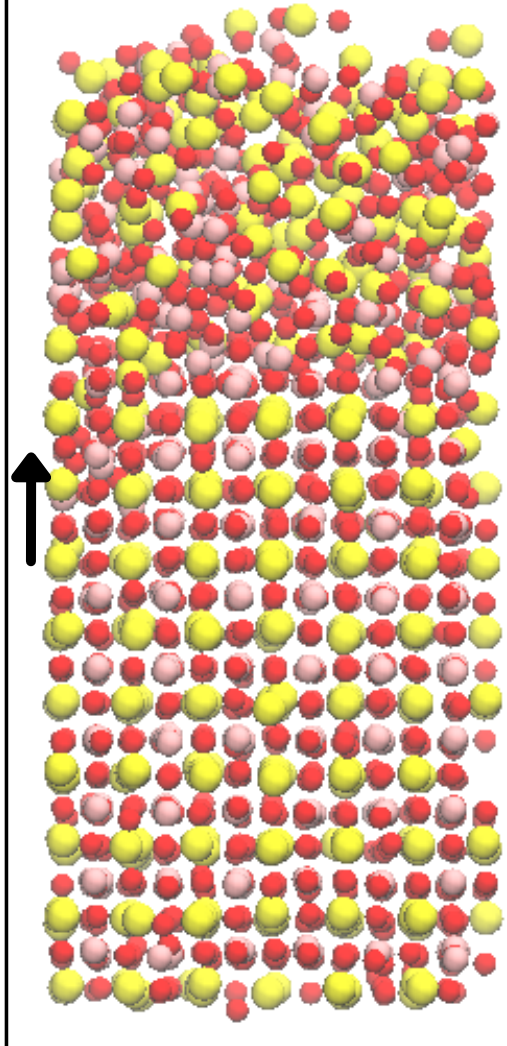


... and a crystal substrate which will guide the amorphous atoms during heating.

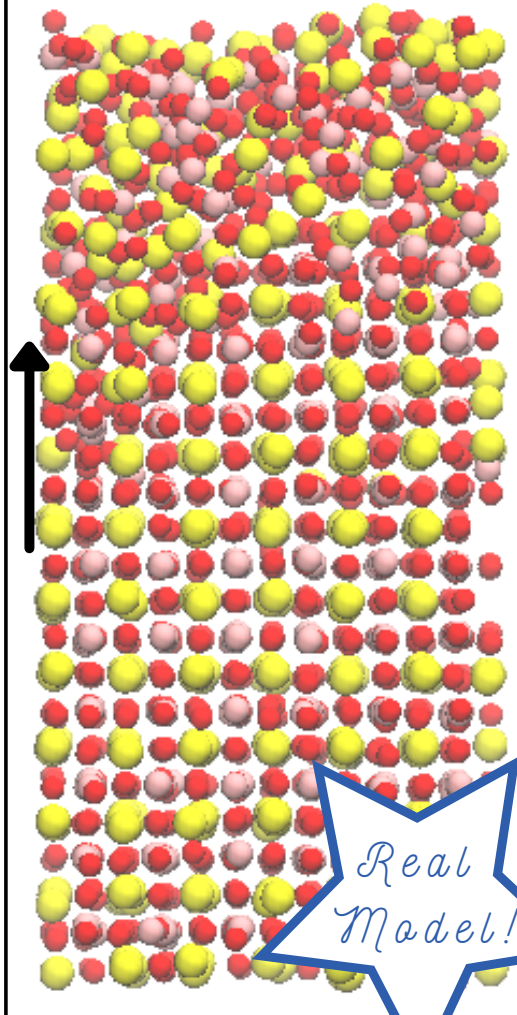
Upon application of a Force Field and heat...



...the amorphous atoms...

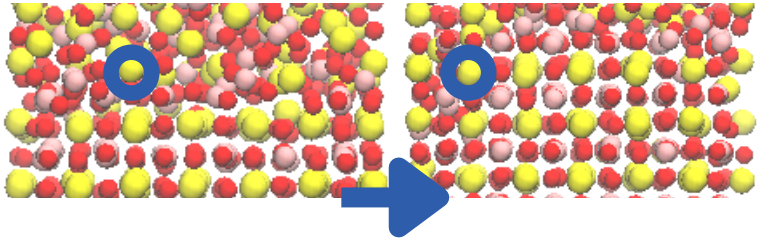


...become crystalline.



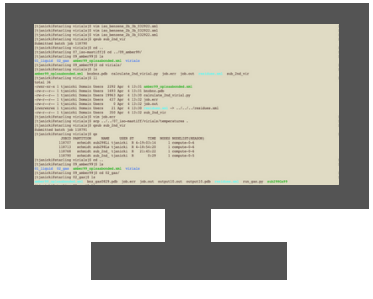
Real Model!

How an atom moved from A to B



Molecular models are important for studying crystallization because we can simulate small atomic motions.

By understanding the mechanism of crystallization with models, experimental methods can be modified to be more efficient and produce more effective nano-electronic materials: quantum dots, semiconductors, capacitors, and more!



Molecular simulations are an essential area of research for understanding how our world works on an atomic level.

Computational capabilities are growing rapidly. It is an exciting time to be a scientist, to ask questions and to seek answers about our universe!

Acknowledgments

Scientific research requires intense collaboration and communication . I am grateful for enriching conversations with my peers and coauthors. I would especially like to thank the following groups for their continued intellectual and financial support:

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Cayce Osborne
Elizabeth Reynolds
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