

# Introduction to Materials Science and Engineering

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# About this Book

This text introduces the core topics and foundational concepts of Materials Science and Engineering. It is structured within the framework of the Materials Science Paradgm. We cover introductory materials processing, structure, properties, and performance with particular emphasis on the relationship between structure and properties. We focus on conventional materials classes: metals, ceramics, and polymers -aand discuss their various properties - such as mechanical, electronic, thermal, optical, magnetic, and electrochemical. Broader themes that arise are how materials' performance influences technological development, the economy, the environment, and society. This text is a pilot version intended to leverage computational tools to assist students in connecting conceptual understanding of materials science-relevant phenomenon with their mathematical models.



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# Chapter 1

## Preface

This text introduces the core topics and foundational concepts of Materials Science and Engineering. It is structured within the framework of the Materials Science Paradigm Fig. 1.1, which focuses in the causal relationship between materials processing, structural, properties, and performance (). We cover introductory materials processing, structure, properties, and performance with particular emphasis on the relationship between structure and properties. We focus on conventional materials classes: metals, ceramics, and polymers - and discuss their various properties - such as mechanical, electronic, thermal, optical, magnetic, and electrochemical. Broader themes that arise are how materials' performance influences technological development, the economy, the environment, and society. This text is a pilot version intended to leverage computational tools to assist students in connecting conceptual understanding of materials science-relevant phenomenon with their mathematical models.

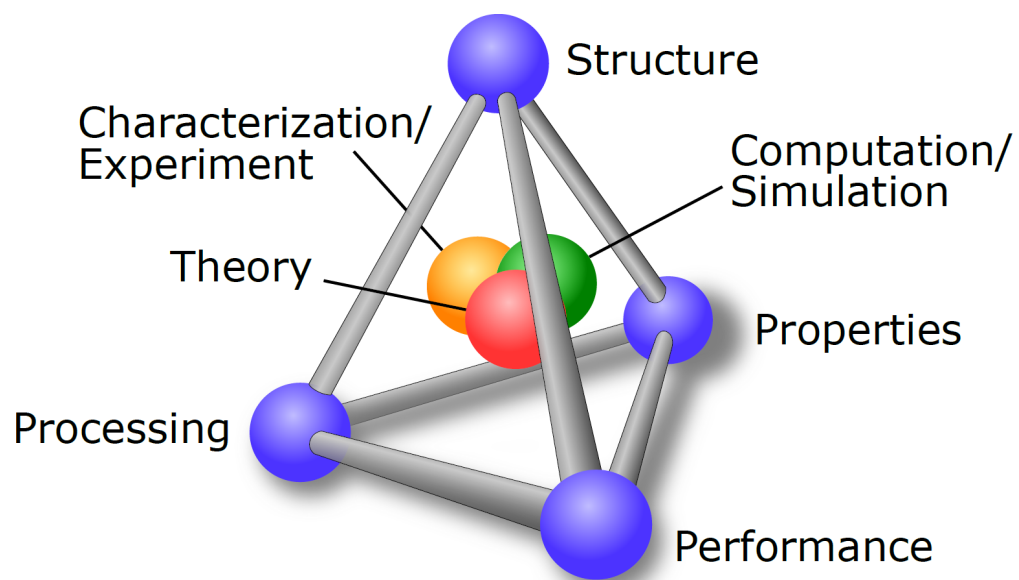


Figure 1.1: The Materials Science Paradigm



## Chapter 2

# Bonding to Crystal Structure

### 2.1 The Atomic Hypothesis

The physicist Richard Feynman opened his famous lectures on physics with the following question: If, in some cataclysm, all of scientific knowledge were to be destroyed, and only one sentence passed on to the next generation of creatures, what statement would contain the most information in the fewest words?

It's certainly an interesting question, and here is Feynman's own answer:

I believe it is the atomic hypothesis that all things are made of atoms — *little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another.* In that one sentence, you will see, there is an enormous amount of information about the world, if just a little imagination and thinking are applied.

There is indeed an enormous amount of information in that one sentence, but let's see if we can make it even shorter. What if we just said “All things are made of atoms — tiny entities that move around in perpetual motion.”? Could we deduce from this short sentence that they attract each other when they are a little distance apart, but repel when squeezed into one another? From simple observations of the world around us, we can. If atoms never attracted one another, then solids and liquids would never form. On the other hand, if atoms didn't repel one another when squeezed close enough together, then matter would collapse into a single point. [lesar2013introduction]

So, we've kept the essential information and reduced the number of words to 14. Not bad! However, our statement is entirely *qualitative*. It won't let us make any predictions beyond what we've already stated: that solids and liquids will form but matter won't collapse. In the coming sections we will construct a foundational *quantitative* model of the atomic hypothesis and see if it is useful. That is, what can we *explain* with this model, and what can we *predict* with it? But first, we will briefly address why Feynman calls his statement the atomic “hypothesis” as opposed to “theory” or “fact” and how we will use models to understand materials.

### 2.2 Scientific Hypotheses, Theories, and Models

When Feynman gave his lectures in 1963, the existence of atoms was scientific fact. Indeed, already by 1908, the biggest skeptics of the atomic hypothesis had finally been persuaded by the evidence [crawford1984arrhenius]. So, why did Feynman call it the atomic “hypothesis” a half a century after it was established as fact? He doesn't say explicitly, but one possibility is that he was describing a thought experiment in which we only can pass on a single sentence of scientific knowledge to the next generation. For that generation, the statement would indeed be a *hypothesis*, as they would not yet have any evidence for it. Based on other parts of the lecture, Feynman also wanted to discuss his view of how science works: in short, we use imagination combined with

evidence to construct physical laws that help us understand the universe. We then perform experiments to test these laws. At the end of the lecture Feynman says: “How do we know that there are atoms? By one of the tricks mentioned earlier: we make the *hypothesis* that there are atoms, and one after the other results come out the way we predict, as they ought to if things are made of atoms.”

Already in Feynman’s time, and certainly today, we can rightfully talk about the atomic “theory” instead of “hypothesis.” In everyday language, people use the word “theory” to mean something more like “hypothesis” (e.g. my theory of why that happened is...). The word “theory,” in physical science is properly used to refer to a set of ideas about how the universe works that have been thoroughly tested and are widely accepted as fact. Of course, scientists are people too and sometimes use the word “theory” in the more colloquial sense, which is pretty confusing.

But what is a scientific theory exactly? The words “theory” and “theater” share the same Greek root “*thea*” which means “a view.” You can think of a theory as a way of conceptually “viewing” nature that allows you to “see” it in a new and powerful way. What truly separates a scientific theory from an everyday theory, however, is that the concepts of a scientific theory are linked with precise mathematical and/or computational representations which are further related to measurements we can take in the real world. This is true of a well-formed scientific hypothesis as well. What separates a scientific hypothesis from a theory is, basically, how much evidence supports it.

We will refer to mathematical and computational representations of specific phenomena as “models.” We build models at every stage of the scientific process. A model can be a hypothesis of how things work. It can also be the application of a widely accepted theory to understand a specific situation. A model is similar to a map. A geographical map represents where things are in relation to one another. The world “presents” the actual geography and the map represents it. (That is, *represents* it in a new way.) The map is not the same thing as the territory it represents, and in order to be useful, the map has to simplify. If it were just as detailed as the real world, it would be just as hard to understand. **All models**, not just maps, are **approximations/simplifications of reality**. The statistician George Box put it this way:

Now it would be very remarkable if any system existing in the real world could be exactly represented by any simple model. However, cunningly chosen parsimonious models often do provide remarkably useful approximations. For example, the law  $PV = RT$  relating pressure  $P$ , volume  $V$  and temperature  $T$  of an “ideal” gas via a constant  $R$  is not exactly true for any real gas, but it frequently provides a useful approximation and furthermore its structure is informative since it springs from a physical view of the behavior of gas molecules. For such a model there is no need to ask the question “Is the model true?”. If “truth” is to be the “whole truth” the answer must be “No”. The only question of interest is “Is the model illuminating and useful?” [Box 1979 robustness]

Understanding this, we might provide a slightly more nuanced answer to the question “How do we know that there are atoms?”: We have constructed models of atoms and their predictions match experiments! However, except for the simplest of cases (e.g. a single hydrogen atom), and using our most sophisticated models (e.g. quantum mechanics), “matching experiments” means only approximately matching.

In our study of materials science and engineering, we will use many types of models including both mathematical and computational models. None of them will represent the “whole truth” about materials, but they will each be illuminating and useful for something. Let’s get started with our first one.

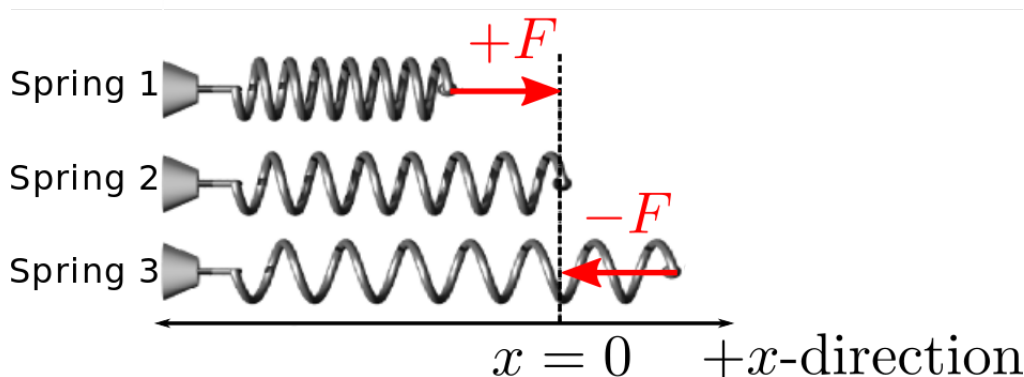


Figure 2.1: Three springs with equilibrium ( $F = 0$ ) positions of  $x = 0$ . Spring 1 is in compression, with restorative force acting in the  $+x$  direction. Spring 2 is at equilibrium. Spring 3 is in tension, with restorative force acting in the  $-x$  direction.

## 2.3 Modeling the Atomic Hypothesis with Interatomic Potentials

When building a model, you first have to decide what the entities of your model will be. In this course, we will typically model atoms as Newtonian objects (i.e. point objects with position and velocity) that exert forces on each other. While this is clearly “wrong”, as atoms (and therefore many of their properties) are quantum mechanical in nature, we won’t worry too much about that at this point. As we move forward, we encourage that you keep mind concepts regarding atomic structure as covered in the Chemistry Review session.

Instead of spending too much time on atomic orbitals and electron configurations, we’ll start with a review of the physical definitions of force and potential energy and then use those concepts to construct our model.

### 2.3.1 Review of Force and Potential Energy

Let’s consider an idealized spring, shown in Fig. 2.1, which is governed by Hooke’s Law. This spring is oriented in the  $x$ -direction, and one end is positioned at  $x = 0$  when in equilibrium. When displaced in the positive  $x$ -direction, there is a restoring force  $F$  acting to pull the spring’s end back to  $x = 0$  that is linearly proportional to the distance the end of the spring was displaced,  $x$ . Similarly, when compressed along the  $-x$ -direction, there is a restorative force acting the the  $+x$  direction. Hooke’s Law is written as

$$F(x) = -kx \quad (2.1)$$

{#eq:hooke}

where  $k$  is the spring constant - a measure of how stiff the spring is. A higher  $k$  means a larger restoring force when the spring is displaced. Fig. 2.1 displays a red (solid) line that follows Hooke’s law eq. ?? as a function of  $x$ .

We relate the force and the potential energy  $U(x)$  as a function of  $x$  by

$$F(x) = -\frac{dU(x)}{dx} \quad (2.2)$$

{#eq:pe}

Below, the  $U(x)$  is plotted as the purple dashed line. eq. ?? says that the restoring force is equal the the derivative of the potential energy function. Intuitively, you can think of the potential function as a landscape that a ball is rolling around in. The ball feels force that causes it to roll downhill. The magnitude of that force is proportional to

the slope at the the position it is located. When potential energy is at a local minimum the force is zero (it is at equilibrium). The further the ball is displaced from this local minimum, the higher its energy.

### Concept Check Questions

Take a few minutes to answer the following questions before you continue.

**Q1.1: Based on Hooke's Law and the equation for potential energy, why is the general shape of energy curve parabolic? Do some math to show us why.**

Potential energy is defined as  $dU/dx = -F(x)$ , so we can plug in the expression for  $F(x) = -kx$  and integrate:

$$U(x) = \int kx \, dx$$

$$U(x) = \frac{1}{2}kx^2 + C$$

This is a parabolic equation. The constant  $C$  determines our reference point. If, for example (and this is a fine idea, here) we decide that we want  $U(x = 0 \text{ m}) = 0 \text{ N}\cdot\text{m}$ , then  $C = 0 \text{ N}\cdot\text{m}$ .

Let's make sense of this intuitively.

1. The potential energy stored in the spring is a function of how far it is from equilibrium. The further it is from equilibrium, the higher the potential energy.
2. In order to stretch/compress the spring, you have to exert a force on it which increases linearly with displacement. As you stretch the spring, the larger the restorative force (the harder it is to pull):  $F(x) = -kx$ .
3. Now let's relate steps 1. and 2. The potential energy of the spring depends on how far it is stretched, and stretching it gets harder and harder the larger the displacement. So, for any little distance,  $dx$ , that the spring is stretched the potential energy should increase more than it did for the previous little distance,  $dx$ . This explains intuitively why the potential energy is super-linear, but to get the exact parabolic shape, you need to do the math.
4. Mathematically, the potential energy is the sum of the force  $F(x)$  exerted on the spring times the displacement that force was exerted through,  $dx$ , i.e. the integral of the force function  $F(x)$  over the displacement:  $U(x) = -\int F(x)dx$ . The negative sign in this equation exists because the we've defined our force as a restorative force. This convention makes the energy increase as the displacement increases in *either* the  $-x$ - or  $+x$ -directions.

**Q1.2: Assume that the spring constant  $k = 1 \text{ N/m}$ , What is the potential energy of the spring when stretched to 1 m? How about 2 m?"**

To find the equation for the potential energy of the spring, we integrate from equilibrium  $x = 0$  to the displaced value  $x_f$  (we've dropped units below for simplicity):

$$U(x) = k \int_0^{x_f} x \, dx$$

$$U(x) = \frac{1}{2}kx_f^2$$

So:

$$U(1 \text{ m}) = 0.5 \text{ N}\cdot\text{m}$$

$$U(2 \text{ m}) = 2 \text{ N}\cdot\text{m}$$

You can confirm this on the graph by setting  $k = 1 \text{ N/m}$  and finding the value of  $U$  at the values of  $x$ .

**Q1.3:** What happens to the force and the potential energy curves when the spring constant is increased? Describe in words after playing with the model.

As the spring constant increases, the slope of the force function increases along the entire domain. This makes sense, the spring becomes stiffer the spring constant increases, and so the restorative force increases as  $k$  increases.

Similarly, the potential energy function (the parabola) appears to “contract” towards the origin as  $k$  increases. This makes sense, a stiff spring will possess more energy at some value of  $x$  compared to a less stiff (more compliant) spring. That is, it takes more energy to displace the spring over each  $dx$ .

### 2.3.2 Sketching A Potential Energy Function for Interatomic Interactions

In this section we’ll introduce a *NetLogo* molecular dynamics model of two atoms interacting with each other. *NetLogo* is a programming language designed specifically for to model the interaction and behaviors of multiple entities, or “agents”. In materials science, these are often atoms or molecules. A molecular dynamics model treats molecules and atoms as Newtonian objects with position, velocity and mass. They accelerate due to forces they exert on one another (and sometimes external forces) and move according to Newton’s laws. The potential energy that results from the interaction of the atoms, and therefore the force the atoms feel from each other, is modeled using a function called an *interatomic potential*. These interatomic potentials come in lots of different varieties - we’ll first explore how these potentials work in a computational model that we provide, and then we’ll later show you some mathematical models that we can manipulate to derive important metrics such as equilibrium bond energies and distances.

In this *NetLogo* model, you will draw the interatomic potential function and see how the atoms react. The video demo embedded below shows how to use the model and demonstrates how you can draw an interatomic potential function similar to the potential energy function for an ideal spring that you reviewed above. For simplicity, the left atom is held fixed and only the right atom moves. You can think of this as looking at the world from the perspective (reference frame) of the left atom. From an outside perspective, both atoms would be moving. The force the right atom feels will be proportional to the slope of the interatomic potential function at its current location.

Your job is to draw an interatomic potential function to model the way you think atoms behave, using the *embedded model*. We have already stated in the atomic hypothesis that atoms repel each other when squeezed together and attract each other when they are further apart. We can also deduce from observation that atoms must not attract each other very much when they are *very* far apart, because otherwise everything would quickly condense into one giant blob.

#### Concept Check Questions:

Now we’ll spend a few minutes exploring the construction of models that will align with the atomic hypothesis. Answer the questions below. In the next section we will introduce a formal mathematical model of the interatomic potential function based on what we observe here.

**Q1.4:** First, construct a spring potential like that in the model below. Make some observations about how the atom behaves at different positions. Which features does the spring model have that fits atomic hypothesis? What is it missing?

Here are some general observations for the idealized spring:

1. If the particle is at equilibrium, it stays put. If we stretch it, it will move back towards equilibrium.
2. The larger the displacement, the larger the restorative force, and the quicker it accelerates.
3. The atom will oscillate back and forth around equilibrium with large amplitude depending on how much energy we give it initially.

The spring potential has a few features that mesh well with our atomic hypothesis:

1. At some little distance they attract each other.
2. When put too close together, they repel.
3. They move around in perpetual motion (when they have a bit of energy, at least).

However, Feynman implies in [his hypothesis](#) that at large distances, there's really no interaction. We mention this above as well - if the attraction was large at large distances, all matter would collapse to a giant blob! The spring potential models *increasing* forces of attraction at very large distances, which is not physical and not consistent with the atomic hypothesis.

**Q1.5: Now, construct an interatomic potential that more accurately models the atomic hypothesis. What is the main difference between your new potential and the spring potential? Make some observations about the behavior of the atomic pair in this potential.**

The main difference in this potential and the spring potential is that we gradually reduce the force of attraction (by flattening the interatomic energy curve) as we move further away from equilibrium. We set the potential to *zero* as the interatomic distance  $x \rightarrow \infty$ . This causes the following effects:

1. When the atoms are close together, the interaction is very similar to the spring potential, there is a strong, repulsive force that pushes the atoms away from each other.
2. There is still a value at which the energy is minimized and the force is zero. This is equilibrium.
3. When the atoms are placed at larger  $x$ , the interaction is very weak and they approach each other more slowly. This is good, because we expect their interaction to diminish at large distances.
4. At very large distances, there is essentially no force ( $\frac{dU(x)}{dx} = -F \approx 0$ ), and therefore no acceleration. This is good! Now atoms that are far enough away essentially ignore each other!

### 2.3.3 The Lennard-Jones Potential

Now that you have worked to figure out what sort of shape an interatomic potential must have, we will look at one of the simplest mathematical functions used to model interatomic potentials. (Note, there are [hundreds](#) of these potentials that serve to model all sorts of phenomena - not just materials. These potentials are used by chemists, physicists, biologists, and engineers to better understand and predict all sorts of physical behavior!)

The Lennard-Jones (LJ) potential, named after Sir John Edward Lennard-Jones, specifies the potential energy between two atoms,  $U_{\text{LJ}}$ , as function of the distance between them,  $r$  (generalized from  $x$ ):

$$U_{\text{LJ}} = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] \quad (2.3)$$

The two positive constants,  $\sigma$  and  $\epsilon$ , can be adjusted to model different behaviors and yield different depths and widths to the potential. These constants are not derived. They are parameters of the model that can be adjusted to fit experimental data. What they represent will be discussed below. Where do the exponents 12 and 6 come from? The 6th power term can be derived from quantum mechanical considerations due to the effect of fluctuating electron clouds. Interestingly, the 12th power term cannot actually be derived from more fundamental theory. It was selected for mathematical convenience and efficiency, but it serves well to model the interaction between atoms (and molecules) from the quantum mechanical phenomenon of Pauli repulsion.

The figure below shows [an interactive graph of the LJ potential](#) along with each of the terms graphed separately. We plot  $+\left(\frac{\sigma}{r}\right)^6$  (not  $-\left(\frac{\sigma}{r}\right)^6$ ) so you can better see which term is larger as well as when the cross-over of the two terms occurs. Use the

graph to answer a few questions about the potential, below (which are also reproduced in your homework). We suggest you spend a bit of time wrestling with the question either yourself or with a partner. Engaging with the questions in this way will allow you to explore the model more deeply and help to improve your understanding. These questions aren't meant to bog you down, however. If you feel stuck after a few minutes, we recommend looking at the answer (toggle the solution button or look at the posted solutions on *Perusall*) to make sure you understand it.

**Q1.6: Which of the terms in the LJ potential (Eq. eq. 2.3) is an “attractive” term? Which is repulsive?“}**

The  $-\left(\frac{\sigma}{r}\right)^6$  term models attraction (note that it is always negative for positive values of  $r$ .  $\sigma$  is always positive). The  $\left(\frac{\sigma}{r}\right)^{12}$  models repulsion and is always positive.

**Q1.7: What happens to the interatomic potential energy as the distance between the atoms gets very large ( $r \rightarrow \infty$ )? Show this mathematically. What does this value at  $U(r \rightarrow \infty)$  mean?**

As  $r \rightarrow \infty$ ,  $U \rightarrow 0$ . This is because both LJ terms have  $r$  in the denominator, so both go to zero at large values of  $r$ :

$$U_{\text{LJ}}(r \rightarrow \infty) = 4\epsilon \left[ \left(\frac{\sigma}{\infty}\right)^{12} - \left(\frac{\sigma}{\infty}\right)^6 \right]$$

$$U_{\text{LJ}}(r \rightarrow \infty) = 0$$

This value of  $U = 0$  is simply convention - atoms that are very far apart would logically have an energy of zero because they aren't interacting in any significant way. A good place to set energy to zero.

**What happens to the interatomic potential energy as the distance between the atoms gets very small ( $r \rightarrow 0$ )? What does this mean?**

Here, we need to compare the magnitude of the attractive  $U_A$  and repulsive ( $U_R$ ) terms as  $r \rightarrow 0$ . As  $r$  gets very small, the term with the larger exponent will dominate, approaching infinity much faster than term with the smaller exponent, in this case, that's the repulsive term  $U_R = \left(\frac{\sigma}{r}\right)^{12}$ . If you'd like to check, you can also take the ratios of limit and find that:

$$\lim_{r \rightarrow 0} \frac{U_R(r)}{U_A(r)} = -\infty \quad (2.4)$$

meaning that the repulsive term dominates. This means that atoms that are very close together are in an extremely unfavorable configuration and will repel each other strongly. This make sense - two atoms cannot occupy the same location!

**Q1.9: The LJ potential (and indeed other interatomic potentials) are constructed such that the potential energy is positive at short distances, goes negative as  $r$  increases, reaches a minimum, and then increase and approach zero at  $r \rightarrow \infty$ . What does the negative potential energy minimum represent?**

This represents the energy needed to break the bond. The system will tend towards the lowest energy state (the potential energy minimum) and form a “bond”. To break this bond you need to put energy into the system to somehow pull the atoms apart. So, if the bond energy is (e.g., for a pair of ions like Na and Cl)  $U_0 = 4.26$  eV, the well will have a depth of -4.26 eV. You need to put in 4.26 eV to dissociate the Na and Cl bond. This is effectively pulling the atoms to  $r \rightarrow \infty$ .

**Find the general expression for the distance at which the potential energy is minimized. We call this the equilibrium bond distance  $r_0$ , and it is the point of at which net force in the system is zero. Hint: how are potential energy and force related, and how would you manipulate Eq. eq. 2.3) to find this  $r_0$ ?**

We want to find the value  $r$  at which  $F = 0$ . We can find the net force in the system by taking the derivative of the potential energy (eq. ??):

$$\frac{dU}{dr} = -F = - \left[ -12 \left( \frac{\sigma^{12}}{r^{13}} \right) + 6 \left( \frac{\sigma^6}{r^7} \right) \right]$$

Now, since we are interested at the point of equilibrium, we set this expression such that the force  $F$  is zero and simplify.

$$\begin{aligned} F = 0 &= \left[ 12 \left( \frac{\sigma^{12}}{r_0^{13}} \right) - 6 \left( \frac{\sigma^6}{r_0^7} \right) \right] \\ 12 \left( \frac{\sigma^{12}}{r_0^{13}} \right) &= 6 \left( \frac{\sigma^6}{r_0^7} \right) \\ r_0 &= 2^{1/6} \sigma \end{aligned}$$

So, if we have some value for  $\sigma$ , we can derive the interatomic bond distance.

**Q1.11: What happens when you change  $\sigma$ ? What do you think we might be able to model by changing  $\sigma$ ?**

What happens when you change  $\epsilon$ ? What do you think we might be able to model by changing  $\epsilon$ ?

The equilibrium distance between the atoms changes. Increasing  $\sigma$  would allow us to model larger atomic pairs. Smaller  $\sigma$ s would model smaller atomic pairs. Increasing  $\sigma$  also *broadens* the well itself, modeling a more compliant (stretchy) bond.

The depth of the well changes when we change  $\epsilon$ . You would adjust this parameter to model different bond strengths.

## LJ-potential Summary

Now that you have spent some time exploring the LJ-potential, let's summarize.

- The negative 6th-term models the attraction of atoms.
- The positive 12th-term models the repulsion of atoms.
- Both potential energy terms approach zero as  $r \rightarrow \infty$ . The 12th-term goes to zero faster as  $r \rightarrow \infty$  which gives the potential its attractive "tail".
- Both potential energy terms approach infinity as  $r \rightarrow 0$ . The 12th-term goes to infinity faster as  $r \rightarrow 0$  which dominates the energy at small values of  $r$ .
- At intermediate distances (typically on the order of a few Å in most systems), the attractive and repulsive terms cancel out, achieving equilibrium (a minimum where  $F = 0$ ) at  $r_0$ .
- At values larger than  $r_0$ , the atoms are attracted (although very weakly as  $r$  increases).
- At values smaller than  $r_0$ , the atoms are repelled.

In all, we have an interatomic potential function for which atoms repel each other when squeezed very close together, attract each other at moderate distances and essentially do not interact at large distances.

In the next section we will use the LJ-potential into a molecular dynamics simulation with more than two atoms and observe some properties of materials that can be explained by the interatomic potential model.

### 2.3.4 Emergent Properties from the Lennard-Jones Potential

The *NetLogo* model below is similar to the one you used earlier, but now, instead of you drawing the interatomic potential, it is modeled by the Lennard-Jones potential. You will see the two atoms with the LJ potential drawn between them from the perspective of the red atom.

Again, in reality, both atoms would feel a force from the interatomic potential and both would move, but for simplicity, we are holding the green atom fixed and just attending to the red atom. The red atom starts at  $r_0$ , the distance which minimizes the potential energy. Use the model to answer the questions below through which you will observe several properties of materials.



### 2.3.5 Evaluating the Lennard-Jones Potential

The LJ potential is a useful model, but like all models, it has limitations. To evaluate a model, we have to evaluate it in light of the purpose(s) it is meant to serve. Often people think that scientific models are only meant to predict, but models can serve other purposes. A model can explain a phenomenon without making precise predictions. For example, the model of plate tectonics explains why earthquakes happen, but we still can't predict exactly when they will happen (we can, however, predict the general areas they will happen based on the locations of tectonic plates). Other reasons for constructing models include helping us reason about phenomena, honing our intuitions, and helping us design technologies. Sometimes there are trade-offs between different purposes of models. Most prominently, the models that are best at prediction are often the hardest to understand, making them less useful for helping us hone our intuitions and reason about a phenomenon.

In reflecting on the model we built we can ask ourselves a couple questions:

- How is this model useful? It holds values because it:
  - Allows us to better conceptualize interatomic interactions.
  - Predicts real phenomenon such as thermal expansion, melting temperature, and simple crystalline packing structures, and dependence of melting temperature vs number of atoms in the system.
- How is this model limited?
  - **Imprecise predictions** The LJ-potential is simple in form, but doesn't capture the precise details of real interactions between atoms, which are founded in quantum mechanics. Scientists and engineers have made some simple adjustments to improve the quantitative predictive ability of the LJ-potential, of course, which better match physical observation.
  - **Unaccounted-for phenomenon** Speaking of quantum mechanics, an obvious limitation of the LJ potential is that it cannot model any quantum phenomenon.

The LJ potential is also ignorant of the existence of electron. This means it can tell us nothing about the (e.g.) electrical or optical properties of materials, as they depend on the behavior of electrons and their interactions with photons. The LJ potential is largely limited to physical and mechanical behaviors of materials.

- **Directional Bonding** The LJ potential can only model bonds that are non-directional, because the LJ potential only depends on the absolute distance between atoms, not their relative orientations. Non-directional bonding does occur in many materials and results in close-packed structures (e.g., solid phases of group 18 elements (He, Ne, Ar...)). However, there are many different crystal structures that form due in part to the influence of bond directionality. The LJ potential will not be able to predict these structures.

In summary, makes it easy to understand and therefore useful for qualitatively explaining and reasoning about various mechanical properties of materials. For this reason, we will continue to use it at various points in the course. However, the simplicity of the LJ-potential means that there are many phenomena it can't explain. For those phenomena, we will need other models.



# Chapter 3

## siunitx Package

### 3.1 TeX Code

```
n(O2)&=\SI{.15}{\mol}\quad\quad&n(Fe3O4)&=\SI{0.3}{\mol}
```

#### 3.1.1 Rendering

```
[ n(O2)&=0.15 mol           &n(Fe3O4)&=0.3 mol ]
```

### 3.2 TeX Code

```
\si{kg.m.s^{-1}}           \\  
\si{\kilogram\metre\per\second} \\  
\si[per-mode=symbol]  
  {\kilogram\metre\per\second} \\  
\si[per-mode=symbol]  
  {\kilogram\metre\per\ampere\per\second}
```

#### 3.2.1 Rendering

```
[ kg m s-1 \ kg m s-1 \ kg m/s \ kg m/(A s) ]
```



## Chapter 4

# mhchem Package

### 4.1 TeX Code

```
 $\ce{CO2 + C -> 2 CO}$ 
```

#### 4.1.1 Rendering

$(\text{CO}_2 + \text{C} \longrightarrow 2\text{CO})$

### 4.2 TeX Code

```
 $\ce{Gluconic Acid + H2O2}$ 
```

#### 4.2.1 Rendering

$(\textit{GluconicAcid} + \text{H}_2\text{O}_2)$

### 4.3 TeX Code

```
 $\ce{KCr(SO4)2.12H2O}$ 
```

#### 4.3.1 Rendering

$(\text{KCr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O})$



# References

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