JEFFREY C. GROSSMAN: How's everybody doing? Good? Yeah. I wanted to start with some inspiration. And so because I love videos, and I think that's a way of inspiring. And sometimes I think if you feel really passionate about something, you can use song and video as a way of conveying your ideas.

I have a good friend, actually, who's been doing that. So I want to show you-- anybody heard of Fog and Smog? OK. Let's show you this little video, just a minute of it.

DJ DAVE: What's crazy to me is like nobody ever talks in person anymore. Like you got Twitter and Facebook and everybody sending text messages. Like nobody's ever sitting down like this and just talking. You know? For all these technologies, we're actually further apart. You know what I'm saying? Hello?

JEFFREY C. GROSSMAN: That's my good friend DJ Dave.

DJ DAVE: (RAPPING) Would you please put your phone down? You're not walking straight. You're stumbling around. You're in public, man. You're being kinda rude, and text messages are not that important.

Excuse me, lady. Could you please put your phone down? You're talking too loud, like nobody's around. I'm sure you'll find a way to hear what you have to say. I don't want to know that much about your day.

I'm standing on line at my favorite cafe, trying to get my coffee, like I do every single day. This dude in front of me is texting up a storm. Thumbs moving like bees in a damn swarm.

I mean, it's none of my business how you spend your time, but pay attention, dude. You're like next in line. He finally gets to the counter and is like, um. I'm like, man, you're hella dumb.

JEFFREY C. GROSSMAN: All right. Anyway.

DJ DAVE: (RAPPING) Could you you please put your phone down.

JEFFREY C. GROSSMAN: All right. So I won't show all the thing. That's actually a good family friend, DJ Dave. I lived in his room for a year, awesome guy, and he's made some really nice videos.

The point is-- this is not quantum mechanics related-- it is a topic near and dear to my heart as some of you know. And I'm sure you're all closing your laptops and putting your phones down, especially after seeing that. But the point is, he's passionate. So what does he do? He conveys his passion in song.

Now, if any of you-- so this is related to the class-- if any of you have an idea that you're passionate about, like say for your final project, and you'd like to do something like that, I would really be fully supportive. I tried to-- some of you may remember my attempts to get you to do that in 3012, and now guess how many people actually did that in 3012? Right, not so many.

But if somebody wants to take a crack at conveying their project in this format, there's got to be a bonus point or two in that just alone. Right? Are any of you are juniors, junior lab? Are you doing that in Van Vliet's class?

AUDIENCE: Yeah, we did it last summer.

JEFFREY C. GROSSMAN: Yeah. So I saw some of those, and I'm like, man, I want that. I think that's really creative and cool. So I see a lot of really cool stuff. I saw a couple of those. They were really great. So if anybody wants to do that, let me know, and I'd be happy to support however I can, put you in touch with Dave if you want or whatever.

OK. All right. Any questions about class products? So I've been talking to some of you about the projects, and if anyone is still interested, it's not too late. But we're getting close to being too late, so please, come talk to me. If you still want to do a project, this would be like the last week I think to get something going.

What I want to do today is-- well, before I start, here's where we are. OK? So what I want to do is continue on our march. We talked about atoms to solids, laid a little of the groundwork. We'll review some of that and then go onto some of the things you can do once you model solids.

I want to do some calculations, assuming that it works, using the nanoHUB interactively together. Because again, there is nothing like calculating the behavior of electrons with friends. There's no better way to create a good group dynamics and interactions.

Computing has the nuts and bolts, a lot of which we're talking about, some of which were not, and then it has sort of the philosophy. Right? And I really tend to agree with some of the things that people have said over the years on how to use computing. And so I just want to bring this in, and I'll come back to this at the end of the term a little bit more.

But Richard Hamming had a number of very interesting things to say about research and about computing. The purpose of computing is insight not numbers. Right? So the computation is only as good as your creativity and your thinking on both sides, what you put into the computer and what you get out.

He also said what are the most important problems in your field? Are you working on one of them? Why not? I love that, and that's very much an MIT ecosystem way, but it's not true everywhere.

But we should always remind ourselves, even if I solve this problem-- so I'd say, my problem is I want to change the bandgap of silicon from indirect to direct. OK? I can do that now, because we've learned how to do that using simulation. So I can probe materials using a computer.

You should still say, why? The point isn't-- you can't just say, why? Well, because it would be useful. Or why, well, because it can make a better solar cell. That's not enough. Right?

It's really how much impact can you have? What is this going to do to the technology you're working on or the science problem you're trying to answer? And taking it those extra steps goes a long way, and that applies to computing, just like any other area of research.

Better to solve the right problem the wrong way than the wrong problem the right way. So choosing the problem that's a related statement. In research, if you know what you're doing, then you shouldn't be doing it. I like that a lot, and that's where computation is a real enabler.

I love experiments too, but I love the world of computation, especially at this scale. Where you can design-- within a limited number of atoms-- you can design anything. You can think up anything and try it. Right? So there's really the phase space is just enormous, and you can really play around and try crazy ideas, random thoughts, and tangents out as you go. Those are often where the best creativity happens.

And then this is it. Right? Machines should work. People should think. So as you go after this class, and you come out, one of the most important things to come out of this is it's always a balance.

When you do computation, it's a balance between your time and the computer's time. And what you'd like to do is create a balance, such that the computer is solving things for you. And you're spending most of your time not solving those things, not wasting your time on things that the computer could do, but rather on thinking about the kind of problem that you're going to make it do. And you'd be surprised how often in computation this balance is not well kept. OK?

And how often you might spend a lot of your time actually spinning your wheels on something that the machine could actually handle. Right? And how much you might think the machine is actually going to somehow solve a problem that actually you need to think about to solve. Or how much more quickly you could solve it, if you just thought for an hour. You might have saved a million hours of computer time. Right? Seriously, so that balance always has to be kept in mind.

And then the one I like to add is Spider Man's uncle, with great power comes great responsibility, because you have now power. You're gaining power. That's what this class is doing to you. You're gaining the power to calculate things like band structures. Right?

And the responsibility is that I want you to know what you're doing. In the sense that you don't just say I'm going to do a bang structure. Oh, here it is. You check, and you're careful about it. Right?

And you understand how to validate the calculations that you're doing against experiment, and you understand how to converge the calculations. You understand how to make sure you understand what they mean. That's the responsibility. OK? So a little bit of philosophy there.

Anyway, OK. We're going to review a little bit, and we'll talk about some properties. We'll come back to this band structure which is so critical to this part of the class. And if I have time, I'll talk about magnetization, but probably, I'll talk about magnetization on Thursday a little. All right? Any questions?

So we've had a rap video, some philosophy, a little bit of an outline. Where else can we go? Right? Things are good.

Rondo, what's up with that? Was that a good decision? No? How many people saw that? I just want to know. OK, so a little more people are--

But you only saw it on a highlight. Oh, you watched the game. All right. Good. Yeah. But they're going to win without Rondo tonight. Anyway, OK. Yeah.

You bump a ref on purpose? Come on. Come on, man. Anyway, I can't spend more time on it. I don't want to do that.

Let's take a walk through memory lane for just a moment, because I want to make sure we all know where we are. Right? We started with this. There were some strange observations by some very smart people. Tell me what those are. We could ask questions like about these on the quiz.

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: Those are electrons. Yeah. That's an electron. Those are electrons. What's this experiment?

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: This one is? What's this one?

AUDIENCE: Collapsing if that happens.

JEFFREY C. GROSSMAN: Why does it collapse?

AUDIENCE: [INAUDIBLE] classical.

JEFFREY C. GROSSMAN: Classical, then it's got to be what?

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: Yeah. It's giving off energy, and it's not going to hang into its orbit. But then quantum mechanics came along and said, no, that's not true. Right? Because what?

It just is. It's the 'It just is" answer. No, because what it said is that the levels of a quantum mechanical object are quantized, and they have to be in those places. And there's no in between, and that's what this is. What's this?

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: Which comes from that same observation. You'd think that the universe, the hydrogen might emit colors in any frequency, but instead only certain frequencies. And it comes from that quantization of those electron levels, and this, somebody already said this. Right? Photoelectric effect. OK?

Now, those are very smart people, and the weirdness kept going. Now, is that guy ordering two drinks at the bar? Why does he have two? Double slit experiment, that was a cool one, and the weirdness just kept going. Right?

Now, it became very clear that matter behaved like waves. If we took this little 10-slide, where we are, quick, what road if we come on, and we turned it into a music video. Right? Anybody want to do that? That's exciting. OK.

It became clear that matter behave like waves and vice versa. OK? And that we had to lose our classical concepts of absolute position of momentum and instead consider a particle as a wave whose square is the probability of finding it, and there it is. And this became our goal, our task of finding that. Right? That's what we needed to do on a computer, and there's a picture of a wave.

How do we do this? How do we describe this? Well, we needed our F equals ma. Right? So when matter is just a particle, we have F equals ma, but now that it's a wave, we needed something different. And from the elements and the bits of pieces of quantum mechanics, which people were putting together, out comes the Schrodinger equation.

And that's our F equals ma, which tells us how to describe the behavior of waves, if they're quantum mechanical, and it was wonderful. It explained many things. It gave us atomic orbitals. It predicted the energy levels of hydrogen.

Remember how wonderful that was? It gave us, basically, the means to understand a whole lot of this. Right? But nature does more than one electron, and it was impossible to solve for more than a single electron. So here's where computational quantum mechanics comes in. OK?

But there was still a problem, and the problem is that we don't have the age of the universe to do our calculations. And so that's how long it would take to currently solve the Schrodinger equation exactly on a computer for like only a handful of particles. Right? Obviously, you could solve it for one or two particles exactly in a lot less time than that, but once you get up to 10, you're done. And so we started to try to take some inspiration, and we looked at this, a guy's back.

And we said, OK, well, maybe that's telling us something. It's telling us a lot, but it's telling us some interesting physics. It's telling us that the ions are a whole lot heavier and slower than the electrons. So we can freeze them out.

So we started to peel away at the Schrodinger equation, and we made it simpler. OK? We made some approximations, and there are basically the two paths that I talked about in those approximations. At the time, it's about 50 years ago, maybe 60, these two paths were fairly distinct.

And the chemists mostly worked on saying, well, here's the equation we have to solve. We can't solve it. Let's make psi something simpler. Let's simplify psi.

And the physicists mostly said, well, let's not think about psi. Let's just change the Hamiltonian. That's h there. Right? And those are two approaches that led to many different models, many different theories, many different theories.

In the theories, in both sides, the effect of these simplifications led to the picture that we call a mean field picture. Which is that instead of having to worry about all these quantum mechanical electrons interacting with each other, we just worry about them as if it's each one is in the field of the others, an average field of the others, and that's called the mean field method. OK? Those are the methods we're using in this class. That's the method we're using.

And then we talked about density functional theory, and the breakthrough there is that trying to keep track of a wave function, let's say, on a grid of a 2 by 2 grid or 3 by 3 or whatever. Well, this is for actually a 2 by 2 by 2 grid, and you have N electrons. Well, if you have N is 1, so 1 electron, you have 8 points you need to keep track of. But if you had just 10 electrons, then you see that you get 10 to the 9th points. OK? This is the problem of using grids to represent things.

And so if you use the density instead, it's just a constant. Tracking the density is much easier, and the crux of density functional theory, which was worked out in the '60s, is that there is a 1 to 1 correspondence between the exact density of the system and the wave function. OK? And we talked about this last time, about how we sit here, because it's a nice compromise between accuracy and applicability. But I want to come back to this, because this is not-- part of the reason I wanted to remind you of this is that it's just always fun to take these walks through memory lane, and it only took us five minutes.

But another reason is that I want to remind you that we are not solving for quantum mechanics exactly. We're not. We cannot. OK? This is what I mean by the responsibility part. OK?

There are some things that DFT can give you, can calculate about those electrons, that are typically very accurate, but there are some things where it's actually quite off. It's an approximation. Does anybody remember where it tends to do well? I did talk about this in the third or fourth lecture and where it tends to do badly. Yeah. Or one of those two.

AUDIENCE: [INAUDIBLE] solids, periodic structures.

JEFFREY C. GROSSMAN: OK. What about the solids, what properties?

AUDIENCE: Bandgaps.

JEFFREY C. GROSSMAN: That would be a case where it falls into the not so well category. OK? So this is pretty important.

AUDIENCE: Lattice parameters?

JEFFREY C. GROSSMAN: Lattice parameters, yes. It tends to do very well for lattice parameters. So how far apart should atoms be, if they come together in a molecule or solid or a liquid? DFT can do very well. It does very well for vibrational properties, vibrational spectrum, the phonons in a material.

It tends to do worse for excited states, like looking at, say, the optical gap or the electronic gap of material. It tends to the approximations that we had to use to get a method that's workable, all of these have approximations, except this. See? We're up to two electrons here. Those approximations lead to DFT not doing so well for the gap. However, as you may have noticed in your homeworks, that's one of the things you have to calculate in your second homework.

So here's the point I want to make. These methods have advantages and disadvantages. They all are approximate. Some quantum mechanical methods can describe some things very accurately and some things not as accurately, and others may have different balances. And as you go down to more accurate methods that can describe more things very accurately, you tend to be able to do less and less numbers of electrons. Right? Limit your phase space to 12, 20 electrons, and you're pretty limited in how many materials you can explore. Right?

Now, why can we still calculate the gap? Well, and this is, actually, there's going to be an addendum to your homework which I'm going to have to-- I forgot to put this in there, but if this is the density of states. OK. Let's say that's the density of states.

By the way, if I asked you what's the gap of this material, what would you say? Yeah?

AUDIENCE: Those are between the first density of states and second density of states.

JEFFREY C. GROSSMAN: Well, that would be true but I need to know one thing very importantly or I cannot answer whether that's the case. What do I need to know? I need to know the position of something here.

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: The Fermi energy, who said that? Very good. Fermi energy, came from over there. OK? Now, if I tell you that the Fermi energy is here. Then, you're absolutely right.

It's the difference-- and in the DOS plots you get on the nanoHUB, these are essentially levels that come out. If it's a molecule, they're levels that come out, and then they're spread out a little bit. So it's very likely this peak height versus that is going to give you the gap. And in the nanoHUB tool, the Fermi energy is always set to 0 for you. OK? But if I don't specify it, you may not know.

Now, is that a semiconductor or an insulator? Is it a metal? Semiconductor? How do you know? You have a feeling?

AUDIENCE: [INAUDIBLE] between the two bands.

JEFFREY C. GROSSMAN: OK. Well, let's say I put it here. Semiconductor? Insulator? Wait, why can I not answer that question? What don't you know?

AUDIENCE: You don't know the scale.

JEFFREY C. GROSSMAN: What if I told you that this was 0.1, and this was 0.2, and the scale is in eV, then what is it? It's a 0.1 eV gap semiconductor. Right? OK? So well, that's like almost a metal, but it's still semiconductor. It's a very low bandgap semiconductor, where actually electrons will probably populate the conduction band just thermally to an interesting probability. Now, if I told you this was 10 eV, what would it be?

AUDIENCE: Insulator?

JEFFREY C. GROSSMAN: Insulator. OK? Now, I'm going to go on. Don't worry, but the last point is DFT, I'm not going to go into the details of why, but DFT tends to underestimate the bandgap. OK? And so there are now sophisticated ways of correcting that and going beyond DFT that we're not going to talk about in this class.

But what we are going to do is we're going to use an approximation that was used for 20 years in the scientific literature and community to correct for this problem. And that is simply called a scissor shift, where basically, you see, DFT gets the bandgap wrong, but it gets qualitatively very often the picture right. It just gets the bandgap too small.

So very often, we just shift the conduction band states by some correction. OK? I will give you that correction. That will be the addendum in the homework, because you'll need that.

So the DOS plots that you calculate for these solar fuels, think of them as pretty good, except you have to shift these states up. So qualitatively, these states are not bad, but they're just too low in energy compared to the occupied states. OK? So that's a method that is not really used very often anymore, but it was used heavily in the '70s and '80s, to use DFT to look at DOS and band structures.

Nowadays, we do have methods that go further that allow us to actually calculate these things without some rigid shift approximation, but calculate them more from first principles. I won't go into those in this class. OK? Any questions? So you'll have to download your DOS plot and do the shift that I give you to the data. All right?

Seems like a cheat, and it actually is a cheat. But like I said the qualitative nature of these states is still very good often. OK? So that's a property DFT does not do so well on.

OK. I won't go through the self-consistent cycle. What we did on Tuesday is we talked about solids. OK? So we talked about the periodic cell, and we talked about crystal symmetries. And this was all review, I think, for most of you, and most symmetries are-- most common lattices are cubic or hexagonal, close back. Anybody know why? Yeah.

AUDIENCE: Lower energy.

JEFFREY C. GROSSMAN: Yeah. Because of what?

AUDIENCE: More atoms.

JEFFREY C. GROSSMAN: You pack them in. Makes sense. OK? And then, and this is sort of where we spent some time Tuesday and I want to make sure we feel our oneness with this k-space thing. So associated with each real space lattice, there exists something we call reciprocal lattice. It's a set of wave vectors which are commensurate with the real space lattice. Sometimes, we call it G. Why not?

Those are the lattice vectors in reciprocal space. And we define them as a star, b star, c star. That's a lattice in real space, BCC, BCC lattice. And there's the reciprocal space lattice. It's a real lattice. It has distances in lattice world, in reciprocal lattice world. It just looks different. And actually, the inverse of BCC is FCC.

So we talked about all this. And then we talked about how you can define a zone within reciprocal space. And the first-- if you take-- if you draw lines between neighbors and nearest neighbors and you draw bisections, then you define that zone. And that's called the Brillouin zone.

And so you see here in this square lattice, it's a square. In here, it's going to be a hexagon. And if we define that zone in three dimensions-- well, here, it's squares and hexagons on the edges. But it's a volume.

Does everybody-- so we're just defining space, still. And then came the Bloch's theorem. And in Bloch's theorem, what we said is that values of a function, like the density, should be the same because it's a crystal. But the wave function is periodic only when multiplied by a phase factor. And that's-- I didn't go into a lot of detail. But that's Bloch's theorem. So it says that the wave function picks up a phase factor, which depends on this new quantum number. That's all review from last week.

And you can see that if the wave function looks like that-- so if you add-- the periodicity of the lattice is big R. R is just anywhere in real space. Then you're going to get this phase factor. And if you square them, say, to get the density, then you can show that the densities are the same.

Also, and this is important, the wave function picks up a phase if you just go by the periodicity of the real space lattice. But if I increase k, if I add an inverse lattice vector to k, then they're exactly the same. So in k-space, I can also translate around. And the energies are the same.

We're going somewhere here. We're going somewhere. Give me a minute. And then I showed you this. And does anybody have questions about this? The parallel here, I think, is pretty self-explanatory.

In the hydrogen atom, we impose this spherical symmetry.

AUDIENCE: [SNEEZING]

JEFFREY C. GROSSMAN: Gesundheit. And we got out of that quantization-- we solved. And here, we impose a translational symmetry. And we get out of that k-vectorization.

We-- but k is not a-- k is a quantum number. But it can be continuous. It can be continuous. And you look at it in the first Brillouin zone.

Now, somebody tell me, given this, why would I worry about k only--

AUDIENCE: Sorry to interrupt you.

JEFFREY C. GROSSMAN: No problem.

AUDIENCE: I'm just videotaping. And we're just hearing the mic move a lot. I'm just going to--

JEFFREY C. GROSSMAN: Oh.

AUDIENCE: There you go.

JEFFREY C. GROSSMAN: So I should stop-- I kind of-- no.

AUDIENCE: [LAUGHTER]

JEFFREY C. GROSSMAN: That rap got me a little bit excited. So let's go back to slide 1.

AUDIENCE: [LAUGHTER]

JEFFREY C. GROSSMAN: So I'm adding an inverse lattice vector, a full vector, that gets me to another lattice point in inverse space. And I say my wave function is the same.

Now, why is it-- I also defined a Brillouin zone. And you can see my definition of the Brillouin zone is, in fact, that it's a zone that-- it's a lattice vector. You see, those are the lattice vectors. Why is it that I only now care about the variation of k within that first Brillouin zone?

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: Yeah?

AUDIENCE: Same thing.

JEFFREY C. GROSSMAN: The same. That's why we care so much about that Brillouin zone. What is it? Well, it's the boundaries of the variability of the wave function in terms of how it depends on k.

So I only need to vary k in this first zone. But I do need to vary it in that zone. I have to vary it in that zone because there will be variation if it's a solid. But if I vary it and then go out here, well, it's just-- I can translate it back. And it's the same thing, you see?

So I need to move k around in this first zone. And when I do, and this is a slide I've showed before-- when I do, what you get is, as you go-- as you think about a system going from atoms to molecules to bands in your solid, you see this is the energy of that band. It wiggles.

That's what happens in that first zone. You have a new quantum number. You change it. And you vary the energy. It wiggles. So now these orbitals are wiggly. And that's the big-- the most important thing.

And you can see here-- so here's my k-space. And I can vary kx, ky, kz if it's three-dimensional solid. And at each point in k-space, you are going to get a set of levels, just like you did for that atom or molecule.

You're going to get a set of levels. And they will vary. But they will be the same if I translate by the inverse lattice vector. So if I go from here out some G vector, then I get exactly the same levels. But if I'm inside this Brillouin zone, they're going to vary.

Any questions? K-space is really important for solids. Mm-hmm.

And so what do we do? Well-- so the inverse lattice-- it's related to the real space lattice. If I double the real space lattice so it's periodic, but with more atoms in the cell-- so it's periodic over a larger domain-- then, basically, I'm-- it's like a Fourier series.

So if I go to larger real space lattice, then I have finer and finer k-space. And so what that means is that you can choose a certain k-mesh. This is a variable in the input now for solids. For solids, this is a new critical variable in your calculations of solids. You need a k-mesh.

And this is just a number. You'll enter 8 or 2 or 4. And it'll just do a cube because it's simple. But you don't have to do a cube. But the code does a cube on the nanoHUB.

So if I enter 8 by 8 by 8, I get 512 k-points on a mesh. And what that does is it allows me to-- it is-- it, effectively, is like increasing how much real space I had because they're related. If I had a larger unit cell with more real space, I'd have finer and finer k-space. And so you can think about these things as being able to go back and forth.

Now, the reason that you don't go to-- and now, well, how many k-points do you need? Well, you need to have enough k-points-- you need to distribute k-points in your Brillouin zone such that-- what? What's the answer? How many k-points do I need? It's my favorite answer.

AUDIENCE: It depends.

JEFFREY C. GROSSMAN: It depends. What does it depend on? Did that come from the back? I love it. What does it depend on?

AUDIENCE: The electrons [INAUDIBLE].

JEFFREY C. GROSSMAN: It might depend on the electrons. What else might it depend on? How many k-points do I need?

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: Yes. Yes. Look at this picture. Let's look back at this picture. Think about this. And now try to think about how many k-points do I need.

AUDIENCE: Enough [INAUDIBLE].

JEFFREY C. GROSSMAN: Exactly. I need enough. Now, what's enough? Well, enough so that you can resolve how the energy is going to change.

So now tell me, if the wiggles are slow and not so much, if the wiggles are like this, or maybe even they're really flat, do I need a lot of k-points or a little bit of k-points? How many? A lot? Just a little bit because there's just not that much variation.

But if the wiggles looked like this, would I need a lot or a little? And so this is the behavior of bands that look like this-- are more sort of metallicy. And the behavior of bands that look like this, the flat ones, are more "insulatorey." And in between-- and we'll see-- on Thursday, we'll talk about how you can actually calculate the mobility from these bands from this

Wiggle. But you can-- how many do you need? Well, it depends. It depends on the nature of the material. But you have to converge that. That's part of that responsibility. Spiderman's uncle knew all about it.

And so this is where we ended. Oh, man. Come on. There we go. This is where we ended. And so you have energy levels in the Brillouin zone. k is a continuous variable. But you don't actually continue it everywhere because it's too hard.

So you just do-- what the computer does is a bunch of calculations at different k-points on the grid you give it. And what you're doing then is you're moving through-- when you give it different k-points, literally, this is what you do. You say, compute the-- what the computer is doing is it's saying, compute the energy levels at k-point 0, 0, 0. Now compute the energy levels at k-points point 1, point 1, point 1.

And you literally just give it coordinates of k-points within the Brillouin zone. And for each of those k-points, it does the calculations. And it finds a set of energy levels, which are different. And those-- and then you fill that in. And you get your curvy bands.

Who's with me? Who's got questions? Anyone have questions? That's the new-- yeah?

AUDIENCE: So at each point, is a distinct number of energy states within the electrons?

JEFFREY C. GROSSMAN: Yeah. Well, each k-point is the same number of energy states. But they can move around depending on where you are in that Brillouin zone. And their "moving-aroundness" is what gives you the band structure.

So in the code, and I did this on the previous slide-- I didn't talk about it. It was the second point. But on the code, you-- each one of these you can think of as occupied by electrons because it's looking at this k-point and then this k-point.

But when you think about the full band structure of a material, that is not how you look at it. You don't have-- you would-- as you keep increasing your k-point mesh, you would have infinite number of electrons in a band.

That is not the case. What you have is the same as before, the same exact thing as molecular states, which is that you can have-- one band can hold two electrons-- one up, one down. That's exactly the same as in a molecular state.

But depending on where you are in the Brillouin zone, the energy of that band now can change dramatically. And that changes everything in terms of properties of material. In particular, what we're focusing on here is optical properties and electronic properties because those are very quantum mechanically, which we like.

Now-- and the Fermi energy is in the code-- we talked about the Fermi energy a little bit for molecules. It's sort of the energy at which you stop filling. It's the energy-- so you fill your bands up to the Fermi energy.

You can just think about it that way. Don't worry about-- so much about whether it's in the gap or where it is in the gap. We don't need to worry about that in this class.

But it is the energy at where-- at which you stop filling. And so you can see that if you-- I have some properties. I thought I had somebody else. But if you were to fill these and the bands-- and these bands didn't stop nicely, like this, but they just crossed over it, what would you have? What kind of material would you have?

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: Yeah. It's a metal. It's a metal. And if you have the bands stop where you stop filling and then there's a gap, it's a semiconductor or an insulator.

Let's do a few calculations. And then I'll come back to structural properties. We are on our favorite place, the HUB of nano. Come on. Yes! We got to that stage.

Launch Tool-- it sounds like a good idea. And this is where we had some issues last time-- not going to kid you. There it is. And we go to here.

Now, let's do a few things. And so this is the same as-- so it's not letting me scroll again. That's wonderful. There it is.

Now, this is the same as the tool that you're using for the homework number 2 to look at molecules. And in looking at molecules, you just select Molecule. But all the code is doing when you look at molecules-- all the code is doing is it's saying, well, whatever you give me, whatever sort of thing you give me, I'm going to put space in my periodic cell. I'm going to put enough space so that it doesn't see its own image. That's all it's doing.

It's still a periodic calculation. It's just putting a whole bunch of space in there. You could choose Solid and do molecule calculations and just make sure that there's space between what you put in.

However, when you choose Solid, then you can see that it's actually entering the coordinates in a different way. It's using a slightly different language.

Has anybody seen this beautiful non-scrolling thing? Man. Oh, yeah. Well, it's good to be challenged. That's fun. So-- you gotta be kidding me. Did you see that coming? Did somebody see that coming?

Should we go back to the-- to DJ Dave? Wait. What if I did Firefox? Is that better? It's the same. That's beautiful. You get the same thing? It did remember me. Now let's close that.

How often does that happen?

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: But what percentage, would you say?

AUDIENCE: [INAUDIBLE]

AUDIENCE: 60% of the time.

JEFFREY C. GROSSMAN: 60% of the time? 60--

AUDIENCE: I feel the nanoHub [INAUDIBLE] are generally not stable for the Macintosh machines and for the Unix--

JEFFREY C. GROSSMAN: Oh, no, no, no. You can't be blaming this on a Mac. This is-- because it's not a Mac.

AUDIENCE: Not a Macintosh.

JEFFREY C. GROSSMAN: Thank you.

AUDIENCE: I mean the software.

JEFFREY C. GROSSMAN: That must be.

AUDIENCE: I think the software is unfriendly for Windows.

JEFFREY C. GROSSMAN: Well, that's a big problem. So here we are. This looks a little bit better.

Now, when you choose Solid-- so now we have-- look at this.

[GASPING]

You can choose your crystal symmetry because it's a solid. And remember those symmetries that you saw? Well, these are those symmetries except now you have to choose a lattice constant.

See, when you did the molecule, the lattice constant was simply big. It was just big so that the molecule didn't fill its periodic image. But now that we're doing a solid, the lattice constant has to be, well, like the lattice constant of the material. And depending on the symmetry of the material, you're going to get different lattice constants.

So if I-- now-- and have any of you seen fractional coordinates before? Does anybody know what this is? So this is actually an important language of solids where, oftentimes-- so with a solid, you have a periodically repeating space that is set by a lattice constant. And so often, it's simpler to think about the coordinates that go inside that space-- the basis, if you want-- as fractions of the lattice.

So for silicon, actually-- for silicon, it's an FCC crystal with a basis at one corner of the FCC and another atom at a quarter-quarter-quarter out in terms of the lattice. This is not at a quarter-quarter-quarter angstroms. This is a quarter-quarter-quarter scaled by that lattice-- does everybody see that-- which is a cubic face-centered lattice. So that's fractional coordinates.

You can go back and forth. You can write a 10-line Python script to go back and forth between the two. But in solids, often we like to think about positions in terms of the symmetry of the lattice. And so that's how we write them.

Now, in this case, I have two silicon atoms. And we're going to ignore everything and just run it. Is that how you guys do it, anyway, you just simulate? It's fun to do that, just simulate, except that you need to know what you did.

Now, that's what I want to ask you about-- is what did I do? Oh, look at that. This is solid. I only gave it two atoms. And yet, because it has the symmetry in the lattice and all that, it knows how to construct a solid. And that's what it looks like. When the computer thinks about it, it thinks about it like that.

Uh-oh. Where's the-- oh, here we go.

Now, key outputs-- it's telling you that it has-- well, these should really be 4. It has four up electrons and four down electrons. That doesn't sound like that many electrons. How come I only have eight electrons in my simulation and I'm simulating an infinite crystal?

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: Yeah. So very good. But how come-- so it's only the valence because that's where all the chemistry happens. We talked about that. But why are the only two atoms? How can I simulate a solid with only two atoms?

AUDIENCE: [INAUDIBLE]

AUDIENCE: Because it's symmetric.

JEFFREY C. GROSSMAN: Because it's symmetric. However, because I only have two atoms, especially, and it's symmetric and it repeats, I need to worry about the convergence of what, which we just talked about?

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: And so you saw-- the density of states we talked about. Oh, this is beautiful. Look at this. It's beautiful. Those are the peaks of the solid of crystalline silicon. It's just like in the molecules.

In the molecules, we had the levels. And we turned them on their side. We turned the levels on their side. And we said that's the same as the DoS. But in the solid, it's the band structure we turn on its side. Here's the band structure.

So those are my levels now. Those are my levels. They're wiggly in reciprocal space. But if I turn-- I can still turn them on their side. And when I do that, I get the density of states, directly comparable to the situation of the molecules. But in the molecules, what I turned on its side didn't wiggle. Does everybody see that? So there's the band structure.

Now, this is-- the nanoHUB has issues with putting Greek letters on plots. So this is the band structure with the Greek letters. And I'll talk about-- well, actually, I don't need to wait. These just correspond to different points in that Brillouin zone.

You cruise through phase space in the Brillouin zone. And you plot the energies-- the code is plotting the energies along that path. So you get a sense of the variation.

Could these energies vary differently than I've plotted here? Could they vary differently? How could they vary differently? The answer is yes.

This is a cruise through phase space. Gamma is always the origin. Gamma's at k-point 0, 0, 0. And then I went to some other k-point. And we called it X. We like to give high-symmetry points in the Brillouin zone a letter, a Greek letter, or not.

And then I went back to gamma. Here, I went to a point we called L. And I-- the way you do this is you just, basically, go in a line from this point to that point. And you plot the change in the energy of each band as you go from point to point in the Brillouin zone. So now, tell me, are those the only variations that you could have? Why not? Tell me why not.

AUDIENCE: If you choose a different path, [INAUDIBLE].

JEFFREY C. GROSSMAN: If you choose a different path. This is just one path going from L to gamma to X. You see, here we are. I went-- you see, here they are for FCC, I think, or maybe it's BCC. I went from gamma to L to X. I went just along a line in this Brillouin zone.

But what if I had gone like this or what if I'd done like this? Would I get different curvatures? You better believe it. You are taking paths through the Brillouin zone to get the band structure. That's how you get the band structure.

Now, what ends up happening is that the interesting variations in these energy bands, the interesting ones, the ones that are important for optical and electronic properties, tend to happen between the high-symmetry points in the Brillouin zone. They tend to happen between the origin and the center of this face and the center of this edge and going back to an origin. They tend to happen between the path of one high-symmetry point to another.

And so, de facto, we just don't care much about everything else in the Brillouin zone because it doesn't really give us extra information. It would give us a different band structure. But it's not that-- it's not giving us something that's as relevant to the key fundamental properties we care about. So that's one thing.

Now-- so that's where those-- now, the code just picks the paths. But in all these codes, you can enter whatever path you want. So if you want to cruise around in k-space and get energy variations, you can do it. You are not limited.

Now, is this the right band structure for silicon?

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: Let's go back to our-- not bad-- looks pretty good. I like that. That's why I want to-- now, if we go back to the input, what is it that-- of these parameters, what is it that I might need to check?

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: What is that? Say that again.

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: So I might-- I have a 4-by-4 grid. Would I get a-- would I get curvy band structures if I do a 1-by-1-by-1? Let's see. Let's try it. I'll do 14.

This seems to be stable for now. Uh-oh, where's my Simulate button? There it is. So I'm doing a 1-by-1-by-1 k-point. This is another key concept I want to make sure we understand.

There it is. There's silicon. I didn't change anything about the real space. I didn't change anything about the k-space. I just only evaluated the density at one point.

Now, here's what's going to perhaps surprise you, which is that the band structure still curves. Now-- and it curves differently, actually, than it did when I had 4-by-4-by-4.

Why would it still curve? This is actually something I didn't talk about yet. But it is an aside that I was going to talk about. But since I have it here, I'll just talk about it now. I probably could have done all that internally without voicing it. But here we are.

So you see, when you calculate the band structure, what you do is you do two things. First, you converge the wave function in density. First, you converge the density at the k-points I input into the input.

So if I have a 1-by-1-by-1 k-point density, well, that gives me some grid. That gives me some density and some wave function.

Now, then to calculate the band structure, what the code does is it does a second step. It takes that converged density. And it cruises around in k-space. And that's how it plots this out. But it doesn't change the density anymore. It doesn't change the converged wave function. It just evaluates it at all kinds of different points in k-space.

So there's two steps. First, you converge the density at some number of k-points. Then you cruise around in the Brillouin zone with that density. And you evaluate your functions.

And sure, the wrong density will still wiggle as you move around in k-space. It'll still wiggle. But it's the wrong density because I didn't have enough k-points in the first place to converge it. Does everybody see that?

So now, how many k-points do I need? Well, the number of k-points I need is when this converges and doesn't change anymore if the band structure-- if properties of the band structure are what I want. That's how many k-points I need. Does everybody see that? That's the difference.

Now-- no. That wasn't good. Here we go. Oh, yeah. These so-called web browsers-- Marc Andreessen was my student, by the way, that-- does anybody know who he is? No one knows who he is. I'm dated.

No. He was at Illinois, where I did my PhD. And I was his TA. And he went and founded Netscape-- good guy. That's not one of my browser options anymore. So what's up with that?

Now, what I want to do now is the following. I'm going to go to one atom. And what I want to know is-- and you can do that. Just like before, you can mess around. One atom-- we'll just leave it at one k-point.

And what I want to know is, am I going to get a band structure with one atom in the unit cell? Oh, there it is. They're kind of far apart.

What do you guys think? That's one atom in the corner of an FCC cell. Will I get a band structure? Just say yes or no.

AUDIENCE: Yes.

JEFFREY C. GROSSMAN: There it is.

Now, why is it curving? Let me ask it a different way. How could I get these bands to stop curving? Just stop curving already!

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: What is that?

AUDIENCE: Larger k-mesh space?

JEFFREY C. GROSSMAN: Larger k-mesh space or other space?

AUDIENCE: [INAUDIBLE] space.

JEFFREY C. GROSSMAN: Why are they curving again? Why are these things curving?

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: Yeah. It has to do with that. But why do you get-- we talked a lot in the last half-hour about how you get this variation in k-space of the band. Why do you get that, again? Why do you get that?

You get it because of Bloch's theorem. I'll tell you that. But why does that matter?

AUDIENCE: It's periodic.

JEFFREY C. GROSSMAN: It's periodic. You got a periodic potential. And so if it's-- so when would you expect the curviness to stop curving?

Well-- or if you don't really have a crystal anymore. This looks a little less curvy. What if I actually made the spacing-- if I changed the lattice constant to 10 and then simulated? What's going to happen then?

That was pretty fast. And look at that. Now they're far apart. They sort of look like-- let's see. There's the band structure. Ooh! I love that reaction there. That was-- that had some meaning in it. Whoever that was, thank you, because I felt a connection.

What just happened? What is this? What are these?

AUDIENCE: Energy bands.

JEFFREY C. GROSSMAN: Energy bands. They are still energy bands-- varying k-space. But they don't vary in k-space. But you-- doesn't mean you can't compute them at different k-points, which the code did. But they're flat, which means they're not really interacting in any sort of periodic way anymore. They're so far apart that the periodic potentials don't really overlap. They don't feel each other.

So what do I have left then? What is it? What am I staring at?

AUDIENCE: Silicon.

JEFFREY C. GROSSMAN: Silicon atom. That's all that-- those are the states. That's-- which state is that?

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: Yeah. But which state is that?

AUDIENCE: 4s?

JEFFREY C. GROSSMAN: It would be if we had all the electrons. So it is a little tough. But we only have the outer four. So it's actually the 3s. 3s, 3p-- our friend, silicon atom, is back. We went from atoms to molecules to solids. And now we just did an atom.

And you see, as I bring those atoms, as I-- so those are the atomic levels of silicon. They don't vary in k-space. A molecule of silicon wouldn't vary in k-space. But as I start to make this thing feel a "repeatiness," then Bloch's theorem kicks in and energies depend on k. And that changes the properties of the material. So that's all really important.

Now, one more thing while we have the tool up-- well, so now we're actually-- we're pretty well-equipped to try a whole bunch of stuff. And we're going to understand what we're doing.

Let me just ask you one more thing. If I look at these inputs-- let's pull up alpha-quartz, let's say. There's alpha-quartz.

Now, if I look at these inputs, what else might you want to think about converging? We talked about the k-point mesh, something not as bad as alpha-quartz. Aluminum-- well, that's nice, one atom.

What else besides the k-point mesh, and you better use more k-points than one for aluminum-- besides that, what else might-- ooh, I just pointed to it-- might I want to converge or make sure is right-- the lattice constant.

You see, I'm just giving this to you because it's there. Where did it come from? Is it the right lattice constant for this choice of theory and basis set? Is it the right one?

Well, you should make sure there are no forces in the system. You should relax your system. And that gets to the point I want to make.

How do you relax a solid, because there's now two things, not one, that you need to care about? Tell me what the two things are.

Well, how do you relax a molecule? When you say optimize structure, what's it doing?

AUDIENCE: Minimizing free energy.

JEFFREY C. GROSSMAN: By doing what? What's it calculating?

AUDIENCE: Energy.

JEFFREY C. GROSSMAN: Which is also called what?

AUDIENCE: Force.

JEFFREY C. GROSSMAN: The force on each atom. And it pushes them along the force until they get to some minimum.

Now, when I have a solid, I have two things. I have the force on each atom, same as the molecule, the force on each atom in the basis, as well as what?

AUDIENCE: Volume.

JEFFREY C. GROSSMAN: The volume, which is set by the what?

AUDIENCE: Lattice constant.

JEFFREY C. GROSSMAN: By the lattice constant. So you need to converge both of those. And, well, in aluminum, there's only one atom in the basis because, you see, aluminum is an FCC metal. So all I need is one atom in the corner of an FCC unit cell. And I can simulate it. But there is the lattice constant that I need to play with.

Now, if I had a more complex solid, like alpha-quartz, which has a number of atoms in the basis, then the relative positions of those atoms may be important. And you may need to relax that. You may not. But it's something you need to be aware of.

And you can go in. And you can look at the forces on these materials. And you definitely have to know whether you're at the minimum in terms of the lattice constant.

So let's do aluminum just because it's here. We'll do four k-points, which is not enough to look at a metal. But we'll do it because it should be fairly fast.

There's the energy. And-- oh, look at that. Isn't that beautiful? It knew to change the color and everything-- very smart, smart tool. And here we go back.

And tell me-- somebody tell me what they think the band structure is going to look like for aluminum.

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: Is it going to be what? Flat?

AUDIENCE: Curved.

JEFFREY C. GROSSMAN: Curved. How many say curved? How many say flat? Good. Look at that. That's curved. That's seriously curved. And if we include-- if we looked at different energies, we'd see even more spaghetti, lots of curvy--

Oh, and look at this. Oh, let's get the DoS. This is so exciting. I forgot about the DoS. There's the DoS near the Fermi energy. Fermi energy is right here.

Is there a gap in this material? No. Should there have been? No because, remember, in a metal, you've got states coming in all over the place from below the Fermi energy and above-- continues across it. That's what tells you it's a metal.

Now, is alpha-quartz-- let's-- that's a nice material. Mostly, I want to simulate it because I think it'll be pretty-looking. And there it is.

Now, is alpha-quartz-- I'm going to go down to 2 by 2. Is alpha-quartz a metal or a semiconductor, or what is it?

AUDIENCE: Insulator?

JEFFREY C. GROSSMAN: Insulator? Yeah. What's one clue to the fact that it's an insulator? What is that?

AUDIENCE: The inflection in your voice.

AUDIENCE: [LAUGHTER]

JEFFREY C. GROSSMAN: I'm that easy to read? Man, I got to work on that. Is it an insulator or a metal? I'll try. Well, besides the inflection in my voice, what else could give you a clue?

Well, look at it. Is it a transparent material? Well, you can't tell there. Ooh, it is pretty. Look at this. Isn't that cool?

See, this is a periodically repeating structure. But the basis has nine atoms in it. It's a more complex structure.

And let's look. Now, it's an insulator. I'm going to totally agree with that. You see right through it.

So you know it's not what? Absorbing in the visible, at least. But since it's an insulator and it has a large band gap, even though it's a solid, what do you think the bands are going to look like, curvy or not so curvy?

AUDIENCE: Not so curvy.

JEFFREY C. GROSSMAN: Not as curvy. They're not usually as curvy.

So here's the DoS. Look at that beautiful band gap. This is a band gap only a mother could-- a father or mother-- that's the beautiful-- and look at this. There's the band structure. And you can see that-- look at all those bands.

Look at all those levels. And they do curve. They do curve. But they're not as crazy-- well, they are kind of spaghetti-like. But they're not spaghetti-like near the Fermi energy or near the gap.

So you look at that. And you're like, insulator, first of all, just because of how big the gap is. And then what we're going to do-- and I still have just 10 minutes for today. But on Thursday, what we're going to do is we're going to show how, when you look at this, you can say, not a very good conductor, certainly not a good hole conductor.

This is where the holes would move. This is where the electrons would move because we're going to get to that a little bit on Thursday.

Band structure is so rich with information. It's a beautiful thing. It's emotional. And if any of you are feeling that, it's OK. I'm touching the mic again. Sorry. It's OK. We're good. Check that. Roger.

So we're simulating solids. You understand about band structures. We've talked about silicon and occupied, unoccupied-- you can get the densities, just like you can in molecules. And as I said, you can calculate the-- you what? You need to find the equilibrium lattice constant.

And so if you just do the calculation at different lattice constants, you'll get a variation in energy. That's what will happen. And you'll get a minimum.

And that'll be the lattice constant that you should run at for your simulations. And that's pretty important. But if you had that curve already, well, then you've also got the bulk modulus, which is pretty cool.

Now, I think that you probably did this calculation using classical potentials. Is that right? You calculated the bulk modulus? So this isn't any different. It's just the-- did you do-- you did periodically repeating structures, right, using classical force fields?

I'm seeing a whole lot of "I'm not sure." Yeah? It's a very "I'm not sure" kind of moment. It's OK. It's OK. Is it-- did you look at solid materials in your homeworks? It's still no, not so sure. Silicon? Carbon? Not so much.

AUDIENCE: [INAUDIBLE] proteins.

JEFFREY C. GROSSMAN: Proteins? So proteins are a bit more complex of a beast, by the way, which you can't really do using-- you can do parts of proteins using quantum mechanics. But it's just too hard. It's too big. You can't do that many atoms to do most full-sized proteins. So that's a great problem to study with classical models.

For crystals, like the two-atom silicon, eight electrons-- are all those crystals in there-- and not to say 1,000 electrons. You can do things like calculate the change in the lattice with-- change in energy with the lattice.

And from that-- well, this is the volume. But that's just the same as the change in the lattice. And from that second derivative, you can get the bulk modulus, which is a very important property.

And this is something I just went through. This was that slide that I talked about. But it was-- really should have been an internal discussion. And where you find the converged ground state density and potential with some k-point mesh that you gave it-- that's what you input-- is the k-points that go into that calculation.

And then for that, you calculate the energies at k-points along all the lines. And some software-- well, step 3 is not really a step. But use some software to plot it.

And you can download the data for this from the nanoHUB. There's a-- I've been showing you the version of the plot that gives you the Greek characters, which is an image. But there's another version that gives you the raw data. It just doesn't put the characters on it. But that will allow you to compare one run to another and download the raw data.

And then calculating the DoS is also a two-step process. You converge the ground state density potential. And then you use that potential to calculate the energies. And usually, you want to do this at a dense k-mesh because the subtle variations-- see, in a molecule, oftentimes, the DoS is pretty clear.

If I turn-- well, I guess I could've just done this. If I turn, say, an atom or a molecule on its side, then I have this. And you use some kind of smearing function.

And so your-- well, that was a bad centering. And so your DoS would look like that. But there'd be bigger peaks where you have lots of states and smaller peaks where you don't have many.

But, you see, now, I'm turning a band structure, and you saw alpha-quartz-- so now I'm turning-- see if I can just show it one more time-- oh, man. Seriously? Oh, it was in another--

I'm turning this on its side now. And that's not as easy. That's trickier. So there's different weights of a band at different parts in energy. And when I turn this on this side, you can get DoS shapes, Density of States, that are-- that have a-- more features in them. And to get all those features just right, you need to use a dense k-point mesh, which is what the code does.

This can be measured. The DoS can be measured experimentally-- can use STM to actually directly measure the DoS.

And we talked about this already. You fill up your electrons to the Fermi level. If there's any bands crossing, it's a metal. If not, it's an insulator or a semiconductor.

If you have an odd number of electrons in the unit cell, it has to be a metal because the Fermi level is going to come in in the middle. Each band takes two electrons. So if you fill up to the Fermi level and the Fermi level is in the middle of a band, by definition, it's a metal-- sodium.

And then here is a picture of diamond. And the thing that I want to, again, emphasize is that from DFT, these characters of these wiggles and of these features are pretty darn good, but this distance is not.

And so what we-- what we're going to do in this class, and we're going to be proud about it, is we're going to just shift these bands up by a rigid amount to fix the gap.

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: That was probably electronvolts. Yeah, it says it here, electronvolts. And here, it looks like-- what do we have, like, a 3-eV gap from DFT? And so that's about half.

Very often, DFT gives you a gap that's about half of the experimental gap, very often, not at-- always, but very often. For germanium, it makes it a semimetal, which it's not.

Does anybody know what a semimetal is?

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: Not quite. Here's an indirect band gap. A semimetal is a cool material. Germanium is not a semimetal, but DFT will tell you it is because of the gap problem.

Here's an indirect band gap material. Which one is it?

AUDIENCE: Silicon.

JEFFREY C. GROSSMAN: Yeah. Sure. Why not? And if it's silicon, this will be 1.1 eV in experiment and about 0.6 eV in DFT. And that's the band gap error. But again, you can shift it. And that's what we're going to do. We're going to be OK with that.

In-- if you switch to germanium, experiment says it's about a 0.6- or 0.7-eV gap, something around there. But DFT-- that's silicon. But DFT will put it here. It'll put this conduction band below.

It has to actually-- it's-- why didn't I draw that right? It's actually-- comes below. So that is a semimetal when you have, basically, its crossings across the Fermi level, but in an indirect-- from indirect states. That's called a semimetal. And DFT will tell you germanium is that, which is not-- but you can still shift all those states up, which we do.

Oh, there's a metal. Oh, look at that, spaghetti. You now know-- oh, and there it is. See, often in papers, you'll see in the literature-- so you're now becoming sort of experts at seeing a band structure and seeing it, really seeing it.

And it's a powerful thing. And there it is with the DoS next to it, you see, because that's just this on the side, which is why you then plot the DoS sideways, often, except that doesn't quite look right.

But anyway-- oh, maybe this-- yeah. That's what it should be.

And then we've talked about this. And we're going to talk about this. We're going to come back to this a little bit when we talk about solar cells. But I have mentioned this a bunch. Certainly, this would be a good third homework set-- is to think about this indirect versus direct band gap problem.

Somebody tell me, again, why silicon solar cells are expensive just so I can go home today and feel really good or really bad because it's bad news?

AUDIENCE: [INAUDIBLE] bandgap.

JEFFREY C. GROSSMAN: Yeah. But why is that-- why does that make silicon solar cells expensive?

AUDIENCE: You have to make them thick.

JEFFREY C. GROSSMAN: Why do you have to make them thick?

AUDIENCE: [INAUDIBLE]

JEFFREY C. GROSSMAN: Yeah, because you've got to get-- you see, you got to get-- I think I had it shown here. Yeah. See, that's easy for a photon to do. I talked about this. Now, here it is in the cartoon.

That's easy for a photon to do. That's easy for a photon to do at different places in energy. And this would be absorbing light. These blue arrows would be the light that come from the solar flux that you're downloading in your homework.

That's where these blue arrows come. And it's easy for those blue arrows to do this. But to see-- the thing that matters is this minimum amount of energy, the band gap of the material that is the lowest amount of energy that it would take to get an electron up from the valence into the conduction bands. And that, in this case, is not vertical.

It's not vertical. It's an indirect gap. Did I have it there? And because of that, it's not very good at absorbing light.

Those photons, those blue lines-- let's get them back here. Those blue lines-- they need help. They can do this. But they can't do this. And to do this, you need help.

So you need some kind of kick. And that means it's a much less efficient process. And absorbing light in that whole region of the spectrum where a photon would need to do this-- that whole region is very inefficient. And yet that's where the sun is. That's where the sun is.

And so you've got to make them really thick. It's inefficient, but not zero. So you make them really thick. So you get that region of the sun. But to make them really thick, you see, you're generating electrons and holes.

And those-- that generation of electrons and holes-- well, that-- then you've got to get them out. You can't just let them stay there. And to get them out, well, you need a good material.

And if they have to go a long ways to get out, which they do because you have to make it so thick because it doesn't absorb light well because of the band structure, then-- where was I, again? No. Then you need it to be a really pure material. That costs money. Otherwise, they'll run into traps and other things.

So what we're going to do is, on Thursday, we'll talk a little bit more about some other properties. We'll talk about magnetism, very briefly show you that you can do molecular dynamics, a couple other things. And then we'll start turning our attention to solar cells.