

MITOCW | 8. Advance properties of materials: What else can we do?

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JEFFREY So we're here, but don't forget about this. And so the quiz is next Thursday. I'm going to send an email out with office hours for extra time. But if anyone wants to meet anytime, just send me an email, please.

This PSET 2, we decided is going to be due the day before on May 9. And that's when your PSET 3 will be posted as well. And PSET 3 will have to do with the things we've been talking about the last two lectures and today, which is what you can do with solids.

Any questions about the plan, the schedule? OK. Right.

Now, there are other practice problems. I'll throw one out from last year's quiz. So that's a practice quiz that I gave out maybe a year ago or two. And then there's last year's quiz, and I'll pull a problem or two out from that, and we'll do one today, and then maybe we'll look at another one on Tuesday.

What I want to cover in terms of the lecture material today is, I want to briefly start with that band structure and caspase, and make sure we're feeling good about it, and then tell you a few of the things you can do. We talked about the band structure, we've talked about how it has so much information. Well, what other kinds of information is there? What can you do with these sorts of properties of solids?

I love this cartoon. "At some point, his theory becomes so abstract, it can only be conveyed using interpretive dance." And mostly it's because of the visuals that I get on my colleagues here at MIT just dancing.

But we're not going to get this complicated, right? So the point isn't for me to do a lecture on transport theory, and tell you all about phonons and go into great detail about these different things. That is, again, not been our point here. The point is to keep relevant and keep pretty applied in this class.

So I'm going to give you just a little hint as to what you can do with the DOS and the band structure. But we're not going to go into great detail. But you can find those details in many places online and in books. And if you come to me, I'm happy to talk about these concepts that we'll talk about.

So the plan is, we're going to do a little bit of review, caspase, feeling good about oneness, all that. And then I want to show you that problem. We'll talk about just one band structure problem that I happened to give last year on the exam. And then we'll talk a little bit about some properties, electron transport a couple of minutes. And then we'll talk about magnetization, and then we'll do some calculations together again, because I think that's been really enjoyable.

Actually, seriously, I always enjoy calculating together. But how many of you feel like that's useful, to do some simulations here in class? One, two, more? OK.

Because please ask questions. This is the time. Because this is where we can, if you have any questions, please stop. And say, I got no idea what you're talking about.

That's OK. I love those. That's what I want to hear. [LAUGHS] Well, that's actually not what I want to hear. But if I hear it, it's fine. That helps me to know where we need to have a little discussion.

Now, this is the concept that we have to be really good in our understanding. But this is really the key of this second part of the second part, if you want, of the class. Which is, we did quantum, we did quantum for atoms, we did quantum for molecules, and now it's all about solids. And the big difference is that when you have a solid, you have over and over and over again, the same atom, or same couple of atoms in your basis. And therefore, the same potential that the electron feels. And over and over again, how many times?

AUDIENCE: [INAUDIBLE] 2?

JEFFREY If I had to give a number.

GROSSMAN:

AUDIENCE: Oh my god, there's a couple thousand.

JEFFREY Well, I'd say more like a couple of 10 to the 23rd thousands.

GROSSMAN:

AUDIENCE: [LAUGHTER]

JEFFREY 10 to the 23rds. If I take a piece of material, this big, this big, even this big. Even really tiny. You got like, 10 23rd repeats of this potential. That's a lot. So it's almost infinite.

GROSSMAN:

And when you have that periodically repeating well that the electron feels, something happens. And the something that happens was this mathematical thing that, who can remember what it's called? It was a theorem, I believe.

AUDIENCE: Bloch's theorem?

JEFFREY Bloch's theorem. And we don't need to know much about Bloch's theorem except the endgame. The key is what it means. And it's a mathematical consequence. It's a consequence of having an electron, and therefore its solution being a wave function that solves the Schrodinger equation.

GROSSMAN:

It's a consequence of having that in the context of a periodic potential. You can't get around it. It's a theorem. So because of Bloch's theorem, you got to have this requirement, if you want to think about it as a requirement, that when the wave function repeats, the properties just repeat.

The density's the same here as it is here as it is here, 10 to the 23rd out. But when the wave function repeats, it picks up this phase. And that phase is a number that lives in k-space, that lives in the inverse space. And that's why we spent all that time talking about what inverse space is, what reciprocal space is, what k-space is.

And that phase is, you can think about it as another quantum number. So the result of solving the Schrodinger equation and getting psi in a periodic potential gives you a new number. But it's very different than these numbers. How is it different? Yeah.

AUDIENCE: The vector.

JEFFREY OK, yeah. Right. These are like 1 or 2 or 1, 2, 0, minus 1, whereas this is a place in space. And what else is really interesting about that vector?

GROSSMAN:

AUDIENCE: It's in reciprocal space.

JEFFREY It's a reciprocal space. Absolutely. Nice job.

GROSSMAN:

You guys did that together, totally. Team effort, man. I love it.

And what else? It's a vector in reciprocal space. What else?

AUDIENCE: Kind of in the Brillouin zone.

JEFFREY OK, well, it doesn't have to be. But we said it doesn't really matter if you go outside of it, because you just loop

GROSSMAN: back. But what about its variation in the Brillouin zone? How can it vary?

AUDIENCE: Anything.

JEFFREY Yeah. This is a vector that can be anything. This thing can be anything. These things, can they be anything? Can

GROSSMAN: I be pi?

AUDIENCE: No.

JEFFREY Or square root of 2, right? So it's a different kind of quantum number. But you see, it has the same impact.

GROSSMAN: Because, what do these things do? What does this do, anyway? What's one of the things that this does? Or this? What does I do? When I change I from 0 to 1, what's one of the things that happens?

AUDIENCE: Moving from, like, s to p?

JEFFREY Yeah, yeah, OK. So let's write that down. Well, let's change n up to here to s, 1s, 2s. And now you just said I'm

GROSSMAN: moving to p. Now, what is this that I'm always just assuming you know, is what that vertical axis is? What is it?

AUDIENCE: Fill energy from lowest to highest.

JEFFREY Yeah. So this is the energy going from lowest to highest, exactly. And so what did changing the quantum number,

GROSSMAN: l, from 0 to 1 do?

AUDIENCE: It moved from s to p.

JEFFREY Yeah, it moves it around. It moves it around.

GROSSMAN:

OK, so you can change the energy, and actually, you can also not change the energy. m doesn't change the energy. It gives degeneracy. But certainly you can change the energy by changing these quantum numbers.

That's what you can do with k. That's what k does. k, which is a result of living in a periodically repeating world, k changes the levels.

It's the same idea. It's very different, but it has the same impact. It changes these levels around. And it's very different because it can do it continuously, as opposed to these big leaps that we have in the atom.

Or in the molecule. In the molecule, there are also discrete levels. And so we got this picture that we came to last time, where you see, k can be a vector. And it can live anywhere in this inverse space.

And anytime you change it, you may change the energy levels. You may change them. So it's a really important thing when you have a solid.

Now, again, if I have a periodically repeating atom, but the distance between them is like, 100 angstroms. What's the impact of k going to be? We did it in class.

AUDIENCE: It's going to be relatively small.

JEFFREY GROSSMAN: Relatively small. Like, almost nothing. Because the whole effect comes from the fact that you have an electron in a lattice of periodic potentials, where they're sort of interacting, where they're close enough that there's some interaction. If there's no interaction, and your atoms are really, really far apart, then it's basically like you just have isolated atoms, sitting in their potentials. And a whole lot of empty space in between.

And then the levels will just look flat as a function of k -space. Doesn't mean you can't vary k . You could still vary k .

But the bands that you get will be completely flat. They'll go back to your molecular level description. So does everybody see that? All right. And we talked about that.

And so then the question was, well, what playground of k matters? And this is something we talked about, but it's really important. So I want to review it here.

So we just said that k is this new index that is a continuous variable, that changes the energy levels. It moves them around. OK, so what does that mean for a calculation, right?

Well, one thing that it means is that when I do a calculation, if an energy level can now do this, as a function of k , then that means I need to actually do my calculation with a mesh of k -points. How fine a mesh do I need? What's the answer to that?

AUDIENCE: Depends.

JEFFREY GROSSMAN: Thank you. On what?

AUDIENCE: How curvy the bands are.

JEFFREY GROSSMAN: Yeah. How curvy are my bands?

AUDIENCE: Pretty curvy.

JEFFREY GROSSMAN: This is pretty curvy. So maybe I need a lot of k -points to capture this. You got a grid. I'm solving for this problem on a grid of k -points, basically.

And if I only have a k -point here and here, well, let's say I have it actually even worse, I have it here and here, I'm not going to really capture the right physics here. So the density of k -points has to be such that you capture the features, in terms of how much these energy levels vary. So let's go back to these two atoms that are very far apart. How many k -points do I need for those?

AUDIENCE: Two.

JEFFREY What if they're really far apart?

GROSSMAN:

AUDIENCE: One.

JEFFREY One. Whoa. All the calculations you've been doing, until we did the solids, everything before that was actually 1

GROSSMAN: k-point. It was at 000. We never varied it. We never worried about it. It was never an index.

OK, so now, if the bands are flat, you could just have one k-point, and you've got the variation of the bands nailed, since they don't vary. So you just need the one. But if they vary a lot, like if I bring atoms together, and they vary a lot, and there's a lot of interaction, then I just need more and more k-points to represent that correctly. OK, so the k-point is something that's now an essential part of your calculation.

Now, that's talking about what you need to get the density right, which is to get the wave function right, which is to get the energy levels right. That's a new component of a quantum mechanical simulation. But then there was this other thing that's actually a little bit separate in a way, which is to visualize that variation. Now, visualizing this variation leads to these plots, which are called

AUDIENCE: Band structures.

JEFFREY Band structures. This is the band structure of the material. Ooh, it's another kind of phase map, for those of you who felt the excitement of phase diagrams in 301-2. This is like a phase map for that electron. It's a really important description of how electrons behave in materials.

Everything going OK over there?

AUDIENCE: Yeah.

JEFFREY It looked like you got hurt. No, you're good. OK. All right, I got a little concerned, but we're over it. [LAUGHS]

GROSSMAN: Sorry.

The phase map is a walkthrough k-space. Now, I just mentioned that you have a grid that you just have to put on here to do the calculation to get the wiggles that may or may not be there. Well, you should take a guess it whether you think they're there, and then you should see, and then you should converge it.

But now I'm taking a walk around in that zone. And the question is, where am I going to go? Well, I'm using 4 by 4 by 4 k-points. So I'm using a grid of 64 points. And I'm plopping it down into this Brillouin zone.

Should I just look at the energies at each of those points? Well, you could do that, right? Ideally, you'd like to be able to visualize this variation all over k-space, at every single point. But why don't we do that? Tell me why we don't usually do that.

AUDIENCE: Would we be more interested in isosurfaces?

JEFFREY Well, that is true, but that's more of a density thing. So that's where you'd want to know the isosurfaces of the charged density. Yeah?

GROSSMAN:

AUDIENCE: Once you know a certain amount, it's repetitive throughout this direction.

JEFFREY OK, that's definitely true. But let's say you didn't know that. I'd like to do the most accurate calculation possible.

GROSSMAN: Let's say I put a grid over this k-space of a million by a million by a million.

Don't do that on the nanoHUB. We'll get calls. [LAUGHS] But let's say I did that.

Now, I've got a million by a million by a million points in here, where each point has a new set of energy eigenvalues. Why can't I just visualize that? Yeah.

AUDIENCE: Would it just take too long to simulate?

JEFFREY Well, it would take a whole lot of time to simulate. What about visualizing it, though? How would you visualize that?

AUDIENCE: [INAUDIBLE] 3D [INAUDIBLE], right?

JEFFREY But see, it's not even really just 3D, right? Because at each one of these points, I've got a spectrum of energies.

GROSSMAN: So it would be making your eigenvalues, each one into a 3D curve. And I want to look at them all. You could do that.

But you got to remember, if I go down to here, you can't just do it within this volume element, right? My eigenvalues might shift up, down in different ways, depending on where I am. How am I actually going to see that? So in a way, what we have is actually a strong visualization challenge. There's sort of a good story here, because luckily, we can just look at a 2D map of this variation and get all the information we need, for almost all materials.

And so, how do you get it a 2D map? Well then, instead of doing the whole of volume, you just walk through the volume along lines. You literally just walk along this line, and then this line, and then down, and then back, and then up.

And as you're doing this walk through k-space, you plot the energy bands, and you connect them together. And you draw lines between those connections. This is the same energy level just moving around, along that walk.

So that seems like an oversimplification, because I'm not going through the whole Brillouin zone by any means. I'm just going through very particular lines in there. And yet it's all we need. And the reason is that most of the things I want to know about a material, most of the things I want to know, are going to come from the variation in these bands between high symmetry points in k-space. So I can go to other points in the Brillouin zone, and I'll get other levels. I'll get a different set of levels. But it's probably not going to add to my knowledge of the material and the properties that I can get.

So for example, I'm very interested in this where this has a maximum, the valence band, and where the conduction band has a minimum, right? And you'll notice, the minimum for silicon is actually not at this high symmetry point x . But it does come along the path to x from another high symmetry point, γ . It came along that path. And there's no place in k-space that gives me a lower point, you see.

So I nailed the thing I needed I nailed it by going from one high symmetry point to another. And that's what a band diagram is. It's a walk through k-space along lines between high symmetry points. And that gives you the map that you need.

And these sometimes look really complicated, but just think, it's saving you a whole lot of trouble compared to all the data you actually could have. But it's giving you what you need. Are there any questions about that? That's sort of the key point here from this band structure.

And we've talked about this, how you get your bands, just like in an atom or a molecule. You get your energy levels from solving the Schrodinger equation. And then you fill them up, using the Pauli exclusion rule, right?

Add a little bit of Hund's rule to it, although that can be violated. Don't tell anyone. And you fill them up and then you're done. And when you're done, you've got your Fermi energy.

Now, it's the same exact thing here in the band structure. You fill your bands up, until you've filled them up with the number of electrons that you had in your simulation. And then you've got your Fermi energy, and then if there's a small gap there, and no bands cross it, it cannot be a what? It cannot be a--

AUDIENCE: Conductor.

JEFFREY A metal. It can be a conductor.

GROSSMAN:

AUDIENCE: I don't know.

JEFFREY It can be a conductor, a semiconductor, or a really bad insulating conductor, also known as an insulator. But it

GROSSMAN: can't be a metal. Because if no bands cross, if there's a gap here between where you filled to and the next place, then it's not a metal. So we talked about that. And that's, certainly if you have an odd number of electrons, it has to be a metal.

And there's a calculation, I showed this last time of an insulator. And we also talked about how this density of states is another really important thing here. And since this is in your homework as well, in your current PSET, I'll get to transport in a sec. I want to make sure we know what density of states is.

Somebody tell me what the density of states of the carbon atom would look like.

AUDIENCE: [INAUDIBLE]

JEFFREY OK, so let's draw. So we had the carbon atom would have 1s and 2s and 2p. And how many would I put here?

GROSSMAN:

AUDIENCE: 2.

JEFFREY OK, and what about the next one?

GROSSMAN:

AUDIENCE: 2.

JEFFREY OK, I'm liking it. And here?

GROSSMAN:

AUDIENCE: 2.

JEFFREY 2? OK, like that.

GROSSMAN:

AUDIENCE: Aw.

JEFFREY Oh, wait, hold on. OK, thank you, like this. Oh, sorry. All right. That would be an open shell singlet. Thank you

GROSSMAN: very much.

OK, now. OK, so what's my density of states over this? How do I do it? OK, yeah.

So I'm seeing people go like this. So this was energy here. And now this is going to be energy here.

OK, what's my next step?

AUDIENCE: Drawing a curve.

JEFFREY Drawing a curve. OK, I'm going to draw a curve. What is that?

GROSSMAN:

AUDIENCE: 1s.

JEFFREY It's 1s. Why not? I've just broadened it. We'll make that 1s.

GROSSMAN:

And what's my next curve I want to draw? OK, sure. And it should be spaced such that it should be the right energy spacing that I get from my quantum mechanical simulations. OK.

And what's next? 2p. Let's make this go out further.

OK, now 2p. Now, how should I do this? Should I make it the same?

AUDIENCE: Or shift it down [INAUDIBLE] energy.

JEFFREY Shift it down.

GROSSMAN:

AUDIENCE: Same.

JEFFREY Same. Is it different than 2s?

GROSSMAN:

AUDIENCE: [INAUDIBLE]

JEFFREY Well, let's see. I had two electrons in each of these. How many electrons could go into 2p?

GROSSMAN:

AUDIENCE: 6.

JEFFREY 6. So I actually have more states there. I have 3 times as many as here. So in a way, if you're thinking about
GROSSMAN: these as sort of a vertical line, that is spread out by some smoothing function, just to make it into a nice, pretty curve, if it's an atom, if it's really an atom, then it's really just a line. It's a delta function.

But then this should have three lines all on top of each other, right? And so if I look at that, it's going to lead to a bigger peak, that has more area under it. Three times as much, yeah.

AUDIENCE: [INAUDIBLE]

JEFFREY OK. So you can fit 6 electrons into this peak. This is what the density of states is, right? It is the density of states.
GROSSMAN: [LAUGHS] It is these levels. It's these levels. OK. Does everybody see that? Now, where's my Fermi energy for the carbon atom?

AUDIENCE: [INAUDIBLE]

JEFFREY Is it over here?

GROSSMAN:

AUDIENCE: No. [INAUDIBLE]

JEFFREY Here?

GROSSMAN:

AUDIENCE: No.

JEFFREY It feels like it should be here, right? We like Fermi energies between peaks, but that's just because we like
GROSSMAN: semiconductors. No, we like metals too, and insulators. They're all good. So where should it be? Does this sound good?

AUDIENCE: No.

JEFFREY Over here? Hmm? Somebody tell me when to stop. Somebody say stop.

GROSSMAN:

AUDIENCE: Stop.

JEFFREY Yeah. OK, now why am I stopping here? So that's my Fermi energy for the carbon atom. Why is it there?

GROSSMAN:

AUDIENCE: [INAUDIBLE]

JEFFREY Well, it's an atom. So let's not think about it necessarily as conducting.

GROSSMAN:

AUDIENCE: It's where you stop filling.

JEFFREY That's the definition, right? Here I filled and I stopped.

GROSSMAN:

AUDIENCE: [INAUDIBLE]

JEFFREY Yeah. So here I filled and I stopped, and here I filled and I stopped. And what the gentleman over there said is,
GROSSMAN: it's where you stop filling, right?

And so here is where I stop filling, because I had this peak of states, right? It's a peak of states, the density of states, that is only filled by 2 electrons, right? Does everybody see that?

So if I had something else, like say, neon, would my Fermi energy be inside the peak?

AUDIENCE: No.

JEFFREY No.

GROSSMAN:

AUDIENCE: It would be just out.

JEFFREY Just outside of it, because I would have filled it, right? Yeah.

GROSSMAN:

AUDIENCE: Besides the change in the location of the Fermi energy, would the density states look the same for nitrogen?

JEFFREY Very good question. It would, actually. In the sense that if you're looking at atoms, a density of states is a little bit
GROSSMAN: of an odd thing for an atom. But I'm trying to explain it in the context of atoms, because I really want you guys to see the connection, and really what it is.

But if you look at atoms, they're nothing more than levels. And those discrete levels become little shapes that you broaden a little. So it would look the same as nitrogen, because in nitrogen, you would have that.

Now, what does that do? Well, it'll change these energy level positions. It'll shift them around.

This may even change. The 1s may go down or up, this may change a little. And then here, you're going to change not the peak, because you still got 6 states, and you still got 6 electrons you can put in there. But you will change the Fermi energy within the peak, because you can fill it by one more.

And just like going all the way back to our first or second lecture, where we had the orbitals of the hydrogen atom. So we had the nucleus and we had this electron that does not orbit. But there it is orbiting. And then we had the 1s, and then we had the 2s.

And remember how we talked about, it can actually make transitions between the two without actually existing between the two. There are some times it has to cross paths, which are totally forbidden. It's sort of exciting, it's like some sort of interesting fiction. That this electron is going on an adventure.

And well, that's what this is, right? There is no state in here, in this energy. So the DOS tells you that too.

That is what's in the DOS. That information is contained in the DOS. There cannot be an electron with an energy where there's no DOS, there's no states to support it there.

So for an atom, like the hydrogen atom or the carbon atom as well, that's fairly obvious, because you had your levels and you knew it. Couldn't be in between those levels. That's the quantization stuff we talked about.

But now when you get to solids, and it's a more messy picture. But it's the same understanding that you get out of it. It's the same exact understanding.

So what you do for atom, molecule, or solid is you take your levels and you turn them over, and you count up the number of states, and that has to be the same. And you get shapes to the DOS. If it was an atom, I just had these little lines here from the levels, and I broaden them.

Now, the levels are no longer flat. If it's a solid, they can vary. And when you turn that on its side, it can be really different, right? But it's telling you the same thing. It's telling you exactly the same thing.

You're filling your electrons up through here. And you're stopping, well, I don't know, is that the Fermi energy? I didn't tell you. But if it is, then you're stopping there. And those are your unoccupied bands, and so forth.

Does everybody see that? It's the same idea. But it's more complicated when you have these curvinesses.

Yeah. Right? We good? Sort of?

Any questions? Thoughts? Yeah.

AUDIENCE: So when you're looking at allotropic systems-- so in this case, you have done-- I'm assuming that the graphite, this would be completely different.

JEFFREY Completely different.

GROSSMAN:

AUDIENCE: And so how does that tie to solving the density of states?

JEFFREY You can write the density of states for any material. And the same concept always holds, right? That you have these accessible places where the electron can be, with some probability of them being there, right? In other words, it's all about how many possible energy levels you have as a function of energy. That's really what it is.

GROSSMAN:

And so, whatever material you have, the density of states simply has the same meaning, but it will look very different. And in diamond, you're going to get a big bandgap, and in graphite, well, it's a metal. In graphene, you have a crossing at one part in the band structure, goes right through what would have been the gap. OK?

And that's why when you do your homework, when you do PSET 5, there are two ways I want you to think about how these molecules absorb light. One way is that they just have some cutoff, below which in energy or above which in wavelength, they cannot absorb light. So that's just a single cutoff. But the other way is to actually use the features in this plot of levels, of accessible states for the electrons, to use this information and weight the absorption of the sun by this. Because that's actually what's really going on, is that the molecule cannot absorb the same at all the wavelengths of light.

Because in some places it can't absorb any light. In some parts of the DOS, there's no probability. So that turns out to have a really big impact. OK. Questions, thoughts?

Now, let me, before I go on, it's OK. I thought maybe we'd have time to look at Intro to Solar, but that would have been ahead anyway. Oh wait, no. Where is the view?

Huh. That's not looking very good. I had what I thought was a nice example of a problem. No. Hang on one second.

Oh boy. Never show anyone your desktop in a presentation. That's a bad idea. But anyway, oh, final quiz.

AUDIENCE: That's last year.

JEFFREY Yeah, that's from last year. Yeah, don't worry. It's in a very safe location for this year.

GROSSMAN:

AUDIENCE: [LAUGHS]

JEFFREY Actually, it's very unsafe, it's up here. Anyway, wait. Where did it go? Ah. Why can't I see it?

GROSSMAN:

AUDIENCE: [LAUGHS]

JEFFREY Here we go. OK, that's the problem I wanted to talk about. OK, so this was a problem from last year's quiz.

GROSSMAN:

AUDIENCE: [LAUGHS]

JEFFREY OK, so your advisor has just spilled coffee on the culmination of your entire summer UROP work. This is not a true story. The prediction of the band structure and of an amazing new material for solar cells. Unfortunately, in your excitement to show your work, you forgot to back up your data. You dropped your computer in a hot tub and you forgot everything you did.

GROSSMAN:

AUDIENCE: [LAUGHS]

JEFFREY So you only have that one printout now stained with coffee. Can you believe it? This is what you got. Nothing else. OK?

GROSSMAN:

Was this material-- you want to put it back together, because you know-- it was 4:00 in the morning, you had had a lot of NoDoz. But still, you're pretty sure you remember it was going to change the whole field of solar, OK? Now, from this, was this material metal, a semiconductor, or an insulator?

AUDIENCE: Semiconductor.

JEFFREY Tell me why. Really? Seriously? Yeah.

GROSSMAN:

AUDIENCE: Doesn't look like The bands are crossing. Looks like the tallest bandgap is just under the 0. I can't really tell. And then it doesn't seem like the bandgap for the bands is crossing, either.

JEFFREY It doesn't look like it? Can you be certain?

GROSSMAN:

AUDIENCE: No. It's also a fuller cell.

JEFFREY Well, you do need metal, and maybe it was a revolution in the metal contact. That wouldn't revolutionize solar
GROSSMAN: PV, but still.

Again, see, we're inclined to want to connect these things up. We're sort of used to staring at silicon, and we think that's going to do that. But I don't know that you have enough information here. I'm not sure you know enough about this to know that this band didn't actually split, and one of them crossed up and went this way.

How do you know? There is one thing you know it's not. There's one of those three you know it's not.

AUDIENCE: It's not an insulator.

JEFFREY Not an insulator. Why not?

GROSSMAN:

AUDIENCE: [INAUDIBLE]

JEFFREY Because you can make out at least that much, that these bands, they're about an EV or two apart. They may be
GROSSMAN: closer, they may overlap. But it is not going to be an insulator, right? But you can't tell. So this a little bit of a tricky question.

You seem to remember that the material would absorb light very efficiently. Reconstruct the band structure plot that would correspond to such a material. What are you supposed to do here? Yeah.

AUDIENCE: [INAUDIBLE] associated with some wavelength or a region of wavelengths alike.

JEFFREY OK, you could certainly do that. And in a way, any band structure above the bandgap is associated with the
GROSSMAN: region of light. Because except for the bandgap, below which you cannot absorb light, as soon as you start having states, you can absorb light. But the key is here. It absorbs light very efficiently. So what do I need to do in here?

AUDIENCE: Put a direct bandgap.

JEFFREY Yeah. You got to put a direct bandgap in there somehow. That's the key. So you got to reconstruct this. And it
GROSSMAN: didn't matter to me where.

And there were all kinds of really creative curves people drew. But somewhere in here, maybe this is going to come down a little and then go down here. And then maybe come in like here, where you can't see.

But somehow, you got to try to make this a direct bandgap material. It's actually pretty hard, because the stain doesn't give you a lot of room. But it's actually, that mirrors how hard it is to do that for silicon in real life. The stain and silicon are deeply connected.

One minute later, you realize that actually, it didn't absorb light efficiently at all, but instead it was a revolutionary metal electrode. Now what would you draw?

AUDIENCE: Overlapping.

JEFFREY Right. You'd cross it up. Maybe you'd try to get a lot of wiggles in here if you could, or just certainly several
GROSSMAN: crossings, so that the electrons don't really see any gap. You can't see a gap. So that's kind of a nice problem.

And you can see, there's not a very long problem. But you've got to know a few things to answer the question about these sorts of topics. OK, so we'll do another one of those next Tuesday, or two.

Wait, where am I here? Let's talk about a few other properties that you can calculate. Again, I'm not going to go into the details of transport.

But this is sort of basic double E or basic physics stuff. If you put an electron in a field, it's going to push it with a force. And so the F equals ma of that. Yeah?

AUDIENCE: I have a question. [INAUDIBLE]

JEFFREY Please.

GROSSMAN:

AUDIENCE: [INAUDIBLE] absorb things that are greater here. It absorbs light that has energy greater than the gap.

JEFFREY Greater than the gap.

GROSSMAN:

AUDIENCE: But don't you want a very small gap for a semiconductor?

JEFFREY For what application? For solar cells?

GROSSMAN:

AUDIENCE: Oh yeah, sure.

JEFFREY So that's a very good point. And who can tell me why you can't have too low of a gap? And I'll talk about this as we move into solar PV.

GROSSMAN:

AUDIENCE: Because I think the barrier's not high enough, and they keep hopping over. [INAUDIBLE]

JEFFREY That wouldn't necessarily be a problem. Yeah.

GROSSMAN:

AUDIENCE: It would probably get saturated with lower energy.

JEFFREY And what's wrong with that, though?

GROSSMAN:

AUDIENCE: You're not going to be able to use the full potential of the cell.

JEFFREY Well, that's what it is, is it actually is what sets the potential of the cell. So this goes back to, and it's a very good question, right? Why not just use the lowest gap possible? And then you'll absorb all the light, or most of the light.

GROSSMAN:

Well, the reason is that it goes back to this picture that when you're taking photons and making them into electrons, what you're really doing is it's again, it's that pumping water analogy. You're giving the electrons energy and pushing them up a hill. Now, in the solar fuel's case, we're using that push to change the molecule's configuration to store energy. In the solar cell case, we're using that push to get just energy, voltage out, right?

So I'd like to not get just a teeny, teeny bit of voltage. I'd like to get it up a hill. Now, if I make my band gap such that I can only push it really, really high, you might think you want that. But then what happens?

AUDIENCE: Doesn't absorb any light.

JEFFREY GROSSMAN: Doesn't absorb any light. So now you have these two competing effects.

AUDIENCE: Small bandgap.

JEFFREY GROSSMAN: To absorb the light. Larger bandgap to give you more potential for yourself.

AUDIENCE: And large bandgap, more potential, small bandgap, small potential.

JEFFREY GROSSMAN: But more light. And there's a sweet spot. And I'll talk about that. I'll talk about that a little bit on Tuesday. That that is two competing attributes of solar PV that limit how much energy you can get from the sun.

So if you put an electron in a field, it's going to move until you hit this equilibrium point where the acceleration is 0, because the force it feels is balanced by the scattering. That's sort of basic transport, electron transport equations. And so you can get an equation for the drift velocity of the electron. Or the thing that we care about a lot is this electrical conductivity, something that you can measure, which is nothing more than the drift velocity times the number density. That's actually a hard thing to separate out, but it can be done in experiment.

And so the current is that, and it's equal to the electrical connectivity times the field. Now, here's the thing. That equation, then, if you just look at these very simple $F = ma$ for an electron in a field, that very simply comes down to this equation. And here's the thing.

That mass, what we want now is, well, what's the electron conductivity in the solid? What's the electron conductivity in the solid? And it turns out that that mass that's on the previous page, that m , it becomes a kind of effective mass of the electron that can be different than just the mass of the electron, the standard mass of the electron. The reason is that it's in this periodic crystal.

Remember, the electron is going to feel this very strange environment when it's in a periodic crystal. And it's going to feel differences in its energy band. And what that does is it changes, actually the effective mass of the electron, as it's in different parts of k -space.

Well, it turns out that that effective mass is directly related to this curvature. I'm just rewriting the previous equation, but now I'm putting in the band structure here. These little v 's are nothing more than the slope of E in the band structure, the slope of the energy in the band structure versus k .

So this is called effective mass approximation. It's an approximation, but it's a pretty good one. The electron feels a different weight to it. It's heavy or light. Think about it that way.

Depending on whether it's in a flat part of the band, where it's really heavy, or whether it's in a curvy part of the band, where it's feeling more light and bouncy. And that changes the connectivity that can be measured. So just from the curvature of these bands, it's a really nice way of getting a sense of how mobile an electron or hole is in a material. All you have to do is you just take an integral over the derivative of the slope, basically, as you go along k-space there.

So does anybody know what a Fermi function is? It's just a wait. But-- yeah? How many of you don't know what a Fermi function is? OK.

So this comes from Fermi-Dirac statistics. It's not in any way critical here. But it's an occupation function. It's saying that at a given temperature, you're likely to have electrons or not at a certain energy.

And so the Fermi function at 0 temperature, F is going to look like this. Where this would be 1, and this would be 0. And the Fermi function is 1 over e to the E minus E_F divided by KT , plus 1 . Where e is where you are in the band structure. e is where you are in the band structure, and you're looking at this as you go above the Fermi energy.

Can electrons be there? Well, at 0 temperature, no. But actually, when you go to some finite temperature, just temperature alone can kick electrons up.

OK, that's what the Fermi function is in that equation for. Because at some temperature, you can actually have a distribution that looks more like this. T equals 0, T equals something.

Now, what's important here? Well, what's important is that when you think about conductivity, you want to know, you see. The difference here between drift velocity and current or connectivity is that you got to know something about how many carriers you have.

And that's going to be temperature-dependent. Does everybody see that? That's why this is important.

Now, but what if my Fermi function is like this? And OK, let's say I have silicon, and I'm going to now plot on top of this, I'm going to use a different color, and plot on top of this the density of states. And let's say my density of states was like this. OK, I don't know if it is or not. And then here's the bandgap. This is my DOS. That doesn't look like a different color at all.

AUDIENCE: [LAUGHS]

JEFFREY GROSSMAN: It's not even close. It's like they painted it yellow on the outside. And seriously, it's totally white. All right, anyway.

So here's my Fermi function. I'm at room temperature, and this is my distribution of electrons. This is the gap. Tell me what's going on here. Somebody explain this to me. Yeah, Sam?

AUDIENCE: Even though there's probability that you can have electrons in that space, because there's no space for them to go, you still [INAUDIBLE].

JEFFREY GROSSMAN: I love it. That's absolutely right. You cannot have electrons there. The Fermi function says I can. In your face, Fermi function, says the DOS. I didn't say that. I would never say that to a Fermi function. But the DOS said it. The DOS said, uh-uh!

AUDIENCE: [LAUGHS]

JEFFREY We got zero probability here, man! You can't be here. So the DOS said, no states, no deal. Go away.

GROSSMAN:

So the Fermi function tried. It said, hey, I got enough energy from temperature to give you a few electrons. And the DOS says, I don't want them. Because they're not at the energy where I've got any states.

Now, what can I do, then, to populate the conduction band of silicon? What can I do?

AUDIENCE: More thermal energy.

JEFFREY More thermal energy. I'm going to run my solar cell at 10,000 degrees. Well, you'll get more and more. And you

GROSSMAN: will start to get electrons in there. But actually, that's not always practical.

AUDIENCE: [LAUGHS]

JEFFREY So how do we get electrons into there? Then there are other reasons electrons come into those states, not just

GROSSMAN: from thermal. But what's one way that we can get electrons in there?

AUDIENCE: Doping.

JEFFREY Yeah. What does doping do?

GROSSMAN:

AUDIENCE: [INAUDIBLE] changes it from energy.

JEFFREY Well, it can change it from the energy. But what might I dope silicon with?

GROSSMAN:

AUDIENCE: Phosphorus.

JEFFREY Phosphorus. Why?

GROSSMAN:

AUDIENCE: Excess electron.

JEFFREY Excess electron, but compared to silicon. Now, if I have an excess electron sitting in my crystal, but really the
GROSSMAN: crystal is still kind of silicony, because I don't have many of these excess electrons. I just have one phosphorus atom every 1000.

So it's really still silicon. But I filled all my electrons up to here. And now I've got one extra. Where does it go?

AUDIENCE: It goes in there.

JEFFREY Goes in there. And now I'm populating it without thermal energy, right? I don't need to work with my Fermi

GROSSMAN: function, I did it chemically.

I put an atom in there that had a spare electron, right? And that is actually, in fact, exactly what happens in real materials. Who knows what it's called when you have an extra electron, or an excess of electrons?

AUDIENCE: N-type?

JEFFREY N-type. Now, what if I wanted holes? What if I wanted extra holes?

GROSSMAN:

AUDIENCE: B-type.

JEFFREY B-type. And what would I put in there?

GROSSMAN:

AUDIENCE: Boron.

JEFFREY Boron. Because?

GROSSMAN:

AUDIENCE: It's an electron.

JEFFREY It's an electron. Now, you could dope it with many other things. You don't have to dope silicon with just phosphorus or boron. It turns out that those are easy and there are some advantages in terms of their processing, and chemically, they can be happy. But there are many ways of doping materials. Many, many ways of doping materials.

GROSSMAN:

And one of the things you do with doping, there are many things you do with doping. But one of the things you do is you get electrons or holes into these bands. You populate them, right?

But this expression is ignoring that. This is just saying, well, we're going to see if there's some thermal energy there, and we'll use that. OK? Yeah. Any questions about that?

Now, we talked about this a lot. So I'm not going to go over this again, that the direct transitions are easy for photons. The indirect ones where you shift where you are in k-space are hard, OK? And that is why silicon is an expensive solar cell.

So we talked about this, and I don't want to belabor the point, because I want to try to get to some simulations, if possible. Any questions about that point, though, the optical transitions? All right.

So the kinds of things you can get. Well, you can get optical properties, right? And you can also get magnetic properties from these densities of states. So we talked about the optical properties. And the optical properties is really the context of your PSET 5, but it's for a molecule.

We haven't talked about magnetism, and I want to come back to it, because I did mention that electrons have spin. And therefore, they also have a magnetic moment. And we call this, just think of it as some constant that we call the Bohr magneton. It has a value.

Well, and if you think about an atom or a molecule, you could just get that by knowing how many electrons are spinning in one direction more than the other, right? So you can just count how many spin up electrons minus how many spin down electrons you have, and multiply that by the Bohr magneton. And that will give you the magnetic moment of the atom or molecule. But what would I do for a solid? Do I still have it?

Yeah. See, there's the atomic picture where I could just count. And in this case, the difference is 3. Right?

But now, I've got a solid. So what do I want to do? What do I want to look at for a solid?

AUDIENCE: Density of states.

JEFFREY GROSSMAN: Density of states. And it turns out that you can plot the density of states for spin up and spin down electrons separately. And they can be different. They can occupy the two spins differently in a more complicated way, but very much same idea as what can happen in and out of them. But it's more complicated as you get these curvy bands and all kinds of other things that can happen in a solid.

So now, you look at the separate density of states for electrons with spin up versus spin down. And that is something that I didn't talk about yet. It's an input parameter in SIESTA that is checked yes by default. And it's called spin polarized, question mark, I think is what it's called.

Spin polarized? I should give the right intonation. And you say yes or no. And you say yes, because that's the default.

But what are you doing when you say yes? Well, what you're doing is you're telling the calculation to allow the up and down electrons to have freedom from one another. That's actually critical. So if you didn't do that, you would be simulating the material with the constraint that the up and down electrons are exactly at the same energies.

So spin polarized, the reason you do calculations that are not spin polarized is because many systems don't have a difference between up and down electrons, right? And they are actually all the same, right? What do I have if I fill this up? What atom is that?

AUDIENCE: Neon.

JEFFREY GROSSMAN: It's neon. And here, every up electron is the same as every down electron for a given state. Everything is the same here. So it's not like this up electron of this p orbital wanted to be there, and the down one wanted to be there.

That doesn't happen for neon. And it doesn't happen for many systems and many materials. But certainly in some cases, and certainly for magnetic materials, that's what causes magnetism.

It's that you have a difference between spin up and spin down. And that as you occupy the density of states, literally you get a difference in the number, right? So that's what causes the magnetism.

So for many materials, there is no spin polarization. Or in other words, there is no difference. Spin up and spin down is the same here, same here, same here. But if it's a magnetic material, what you'll find is that if you plot the density of states separately for spin up and spin down electrons, like in this case for iron, there's a difference. And in fact, the magnetic moment of that material is nothing more than the integral of that difference.

Again, you're integrating the DOS. And you're finding something really cool about the material. So that's the same thing as just counting number of up a number of down, but now you're counting it in this very complex filling of states that happens in a material. Any questions?

So if I did a calculation of iron with spin polarized checked no, then you see, these would be identical. And I'd get no magnetism. And you can do that. You can actually do the calculation of iron with spin polarized checked no, and it's completely wrong. It's not the ground state of iron.

And if you do it with spin polarized on, then it allows those up and down electrons to move relative to each other. And the outputs, you'll see that in the plots, there's something called the projected density of states. And it's projected for one spin and another spin.

And that would allow you to calculate the magnetic properties of materials using the nanoHUB tool. And I think last year we might have done a homework on that. But this year, we won't.

But I want you to know about it, because it's kind of cool. OK? Any questions? Mm-hm.

A couple other things you can do, and first principles, quantum molecular dynamics, you can do it. You can do MD, just like you did MD in the first part. You're just getting f from the Hellmann-Feynman theorem, which I referred to a couple lectures ago.

But it's basically just a way of getting the forces using quantum mechanics. And I don't really want to go into it in detail, but I just want to tell you, you can get the force on these atoms from these quantum mechanical simulations. And you can do dynamics.

Here's one I did a long time ago. And here the problem was that, how do nanotubes grow, which was a big question, OK?

And so what you have is, you have a piece of iron here. And this is what happens when you grow nanotubes, is you have these seed particles, like iron. It can be other things, nickel, other things will work. Not gold. And then you flow some kind of gas over it that dumps carbon onto the catalyst.

Now, the problem is that understanding how that then leads to the growth of a tube is still an open question, by the way. Still an open question. Nobody actually really knows the full answer to that. But certainly, people were just debating, does the carbon go inside the catalyst or not? Does it stay on the surface, does it saturate the catalyst first, and then come out from the bulk, from the particle?

And that's a perfect problem for quantum, because there's so many different bonding environments, and so many possibilities here, that classical potentials will fail. They're not going to capture all of the different complexities in how carbon needs to bond to iron, inside and out. And so it's a great problem for quantum mechanics.

And we studied this, and we fed the simulation carbon, and we just watched how the tube winds up making its way out of the system. And we showed that it doesn't saturate, actually, inside the iron, but rather stays on the surface. And it makes for cool movies.

Somebody tell me something you notice about this. Besides just, it's kind of a fun movie. But do you notice anything?

There's the initial nanotube growth. And that's where it ended. So I notice two things. Yeah.

AUDIENCE: Some rings are more than 6 carbons.

JEFFREY GROSSMAN: Oh yeah. Actually, that's a really good point. So that was a very interesting part of the analysis is, what kind of carbon you get.

When you catalyze carbon on a surface, what does it do? Does it form nice graphene and then curve it? Or does it form the defects so that you can curve it? Where are the penalties in energy coming from?

But actually, I was going to say some negative things, two negative things. They're not negatives, but they're limitations. Tell me something obvious about this compared to, say, the protein simulations we did in the first part.

AUDIENCE: Very small.

JEFFREY GROSSMAN: Yeah. This is really tiny. And how long do you think this went?

AUDIENCE: [INAUDIBLE]

JEFFREY GROSSMAN: What is that?

AUDIENCE: When was it found? What year?

JEFFREY GROSSMAN: I'm not going to tell you, because that would make me feel old. A while ago. [LAUGHS] But anyway, how long can you run a molecular dynamics simulation having to do quantum mechanics at each step?

AUDIENCE: Very short period.

JEFFREY GROSSMAN: Yeah.

AUDIENCE: [INAUDIBLE]

JEFFREY GROSSMAN: Well, how long could you do proteins with classical MD? Huge systems. Could you do them for seconds? No. But how long?

AUDIENCE: Milliseconds?

JEFFREY GROSSMAN: Yeah, actually even longer. With classical MD, you can get up to microseconds now. Certainly nanoseconds, just 10, 100 nanoseconds, no problem. Here, we're at 10 picoseconds, right? Even 2 picoseconds.

Nowadays, you can push 50, 100 picoseconds, but you wouldn't go further than that. It's really hard. So the time and size are really limited. And that's why with quantum MD, you study small systems for short timescales. This was now cluster growth.

I think quantum, these are just other things you can do. This is supposed to be just making sure you see that it's not just the band structure in DOS. There are other things. You can do a lot of things with quantum simulations.

Water is a really cool problem. And I love Cavendish. I love reading about Cavendish. Has anybody read about Cavendish? He's such a fascinating guy.

He's a university dropout. He compared the connectivities of electrolytes and expressed a version of Ohm's law way ahead of time. And he measured the gravitational constant. And he came up with really water, which at that point was phlogiston and dephlogisticated air, which I love those names. Which is hydrogen and oxygen.

But anyway, water has these really interesting properties. This is a wonderful website to read about water. I'll give you the answer. It actually looks like this.

Water sees water like this, not like this. So it really sees it much more spherical than we usually draw it. And yet, it does have these very definite bondings that it likes to do.

And the point I want to make is, when you go into an MD code, and you put water in there, did you use water in your protein simulations? Yeah. Which water did you pick? You must have picked a potential, or the code picked a potential. Right? Tip 3P to 4P. Well, there's hundreds of them. These are just a few water potentials.

Why are there so many? Well, because some of them reproduce some things better than others, right? And that gets to be a really serious problem if you want to study some of the fundamental problems of water. And there's so many mysteries that we still don't know, in terms of what happens when water evaporates, freezes.

And so, which one is best? Well, this is a perfect problem for quantum mechanics. And I won't go through the details. But you can do water with quantum. And this is a good way to validate which potential you use in your classical simulations.

You can also calculate phonons. You can just displace atoms and calculate energy differences, and get frequencies. So you can calculate phonons. And when you calculate photons in a crystal, that's different than in a molecule. When you calculate phonons in a crystal, you're getting the, waves the sound waves. You're going to get the acoustic waves in the material, right?

You're just using water. In a water molecule, how many phonon modes do I have? In a water molecule? Who can tell me? Take a guess.

AUDIENCE: 6.

JEFFREY GROSSMAN: It's a good guess. Let's get rid of translational and rotational. How many waves can the water molecules stretch?

AUDIENCE: Two.

JEFFREY GROSSMAN: Yeah, there's actually three, right? Because the OHs can stretch, and the bond can stretch. But then there's two different ways that it can go, right? And so those are your phonon modes for the molecule. It's just stretch frequencies, right?

And they can be measured. In a solid, you calculate your phonon modes by moving atoms around in the lattice. And that actually gives you the behavior of the sound waves in the material, which tells you something about how sound travels in the solid, and you can calculate the sound velocity, you can calculate thermal transport. You can calculate the heat capacity of the material.

All of this are things that we do with quantum mechanics that we're not going to do in any of our problems, or anymore. But I just wanted you to be aware of some of the things that people do in research, and that are really a big part of quantum mechanical simulations.

So those are some of the properties. So that was sort of the point here. You can do a wide calculator, a wide range of properties.

This has been our focus, these two. And we're going to stay with that focus. But there's a very large range of things you can do.

Now, I want to just end. I got 5 minutes, OK? And we'll start solar with this on Tuesday. But for five minutes, I want to do a simulation.

So we'll start solar on Tuesday. But here we are. You know which tool it is. It's our favorite.

AUDIENCE: Are we [INAUDIBLE] Tuesday, or no?

JEFFREY GROSSMAN: And we'll do another problem or two in class. And I can do a little review. I sort of did that on Tuesday of this week.

Does anybody want to do more review next week? What do you guys think? A little bit? Yeah? OK.

What I'll do next Tuesday is we'll do another quiz problem from last year like we did today. I'll ask if you have any questions about this practice quiz but, I'll also post the solutions. And I'll go over some key things to keep in mind for the quiz.

So we'll spend the first half of class on that, then. But let me just spend the last few minutes here. Let's do a simulation.

AUDIENCE: It's open notes, right?

JEFFREY GROSSMAN: It's open notes. Open notes, yeah.

AUDIENCE: Does that mean computer is open?

JEFFREY GROSSMAN: I think no. Because that's like, everything, right? What did you guys do in the first part?

AUDIENCE: We had the computers.

JEFFREY GROSSMAN: You had the computers?

AUDIENCE: We had the computers, but we weren't allowed to use the internet. So I don't know how they were checking that. But I [INAUDIBLE] my computer, so I don't know.

JEFFREY GROSSMAN: OK, let's put it this way. If we do open computers, then I'll make the problems harder.

AUDIENCE: No.

JEFFREY GROSSMAN: OK. [LAUGHS] All right. Because Wikipedia's pretty powerful, right? And Google.

And so if you have that, you can find a lot of close answers with a quick search. So I'd have to be a little more creative. But you won't need your computers. And it's full open notes, right?

OK. Now here's what I wanted to do. OK. Let's go to our favorite thing here, SIESTA. There it is.

So I wanted to show you first of all, this feature here, which is that spin polarized. Do you see? Yes? No. OK?

Now, when it's yes, and I calculate silicon, here's the calculation of the density of states of silicon, is what I want to show you. What you are going to find. Oh, I didn't fill out the structure. Is that, OK, so this is just rounding out our SIESTA understanding of what the tool does.

Because there were just these few things that we hadn't talked about. This is the density of states. And you now really feel your oneness with this. You know what these are. You look at this, and you get emotional, which is OK.

But look at this. I also have here, because I did, let's see if it does this right. Total, and there. Look at that, OK.

You see, it's automatically doing what's called the projected density of states. And what a projected density of states is, is it's the density of states, but only for a certain part of the system. Which turns out to be really interesting. Like sometimes you just want to know the density of states for one type of atom. Where is that atom contributing to the states?

Or in this case, because it has been polarized, it's giving me the density of states for spin down and spin up separately. And look at this. They are, while spin down, spin down, you can't see it.

There's some spin up in there. They're exactly on top of each other. What does that mean?

AUDIENCE: Same energy.

JEFFREY GROSSMAN: All the spin up electrons when they're paired with spin down, they all have the same energy. They have the exact same position on this. And they lead to this total DOS here. They just add up.

So if I did silicon with spin polarized off, then the answer would be exactly the same. So there was really no need to do it with spin polarized, but it's the default. And now if I do iron, you see?

And I press simulate. Then what you'll find is that you should see a difference. Let's see if we do.

Here is iron. And now you have the total density of states. Oh, what is this? I forget, is this an insulator?

AUDIENCE: No, it's a [INAUDIBLE].

JEFFREY GROSSMAN: How do I know?

AUDIENCE: [INAUDIBLE]

JEFFREY GROSSMAN: Because I got some DOS here, right? At the Fermi energy. Oh, we got to do it for iron. And now look at this. This is beautiful.

OK, so this is the total, the green. That's the total. And look at this. The red is the spin down. And the blue is the spin up. And look at those differences.

What does it mean? Whoa! I mean, you've got to integrate it to know. But there's a difference.

There's a big difference in the spin up and spin down electrons and where they sit in energy space in the magnetic material. There can be. That's what makes it a magnet.

And so if you integrate that difference up to here, well then, you're going to get this magnetization. If I simulated iron with spin polarized turned off, it would force those to be exactly the same, and they would lie exactly on top of each other, just like they just did in silicon. But that would be not iron.

So you got to be aware of what this spin thing is, and when you need it, when it's important. Keeping it on is safe. But I wanted you to know what it means. So OK. Very good. Have a good weekend.