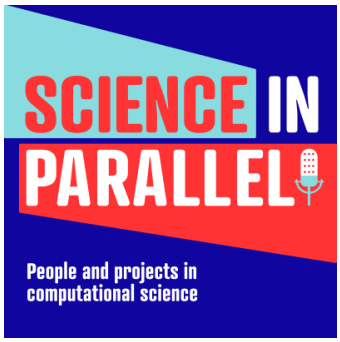

Season 4, Episode
Anubhav Jain: Hacking Materials

SPEAKERS
Sarah Webb, Anubhav Jain

Sarah Webb 00:07
I'm your host, Sarah Webb. And this is Science in Parallel, a podcast about people and projects in computational science. This episode wraps up our season-four series on creativity and computing. And I'm speaking with Anubhav Jain, a staff scientist at Lawrence Berkeley National Laboratory. Anubhav uses machine learning and other computational tools as a material scientist to discover compounds that can store energy to solve other societal problems. Anubhav's current research started in graduate school at MIT, where he was supported by the Department of Energy Computational Science Graduate Fellowship. We discussed how computational tools, including AI, shape the search for novel materials, how he applies machine learning tools to other tasks such as mining data from scientific papers, and the rewards that came from starting his blog called Hacking Materials.

Sarah Webb 01:05
Anubhav, it's great to have you on the podcast.

Anubhav Jain 01:08
Yeah, great to be having this conversation.

Sarah Webb 01:10
So to set the scene for all of this, I want to hear a bit about how you got into material science and into computing. Can you give me a foundation of where these interests came together for you?

Anubhav Jain 01:24
In material science it's always interesting to hear how people get into it because it's not one of those topics that you learn about in high school and in terms of like physics, biology, chemistry. So everybody has to discover material science in some sense. For me, when I was taking chemistry in high school, there were a couple of pages in the chemistry textbook that were more about material science topics. So things like, why is Kevlar such a strong material? What is it about the polymer bonding and the chains that make it so strong? Or how does a hydrogen fuel cell work and, you know, what was needed in the hydrogen fuel cell to make it more efficient, and maybe power cars through electricity in the future versus having them powered by gas. So I thought these pages were really, really interesting. And it motivated me to take an intro to materials science course in college.

Anubhav Jain 02:11
I majored in physics. But I took these intro courses to material science, and I always kind of had it in the back of my head. But I ended up taking more and more material science courses as I went through college. I even did an undergraduate project in material science. So that kind of motivated me to switch to material science when I went to do my Ph.D. And it's been a great adventure ever since. Because it really is applying chemistry and physics and things to real societal problems and energy applications and things like that. In terms of computing, I got started in computing back in second grade, you know, we got the old computers, the 486s, if you are from that era. So I started learning QBasic from my dad,

and you know, just started to get kind of addicted to programming and making little computer games the way a lot of kids, I think, get started with computer programming. And I just kept it up and took AP computer science in high school and things and then also took a lot of computer science courses in undergrad as well. By the time I got to grad school, I was well on the track of doing computer science and materials science topics.

Sarah Webb 03:09
Talk with me about your work at Berkeley Lab and the things that you focus on. Set up the core problem for me. Why is this work important? And how have you chosen to attack it?

Anubhav Jain 03:21
There are a lot of problems in society that would benefit from improved materials. So, for example, for water purification. If we had better catalysts, let's say to remove pollutants from water, that could be new ways of actually filtering water. For electric vehicles, if we had better battery technologies, we could maybe make electric vehicles cheaper and have longer range than they do today. Everything that we touch, everything that we interact with has some materials in it. And if we could improve the properties of those materials, those things would be better. So traditionally, new materials have taken a very long time to develop, there's a paper from the 1990s that says even if you've discovered material in the lab it takes about 25 years to commercialize that material. It's very similar to pharmaceutical development.

Anubhav Jain 04:04
It's just a lot of work to identify the materials as well as to commercialize it. So my group really focuses on how do we accelerate this process of discovering new materials and, ideally, reduce the time to commercialize them as well. And the idea is to use supercomputing and virtual modeling of materials as well as machine learning to make that process much, much quicker so that we can identify the next battery material, the next waste heat energy conversion material, the next water purification materials much more rapidly than if you'd use normal procedures to do so.

Sarah Webb 04:34
So you've been working on these types of problems since graduate school, and I want to get a sense of maybe how the field has changed. How did you approach this problem then versus how you approach this problem now?

Anubhav Jain 04:47
Things have changed quite a bit. When I started, it was a very new idea we were doing almost for the first time with my Ph.D. project, which was to use a whole bunch of supercomputers to screen new materials in a computer. So rather than having an idea, going in the lab and trying that idea out and seeing if it worked or not to actually before you go in the lab to actually screen a whole bunch of materials inside of computers first. And even when people did this sort of modeling of materials properties, they typically did it one material at a time with handcrafted calculations. So what we were doing was trying to automate this process of even just setting up the calculations and running them, and then also scaling them to large computing clusters. Instead of studying just one material on the computer, we could actually test tens of thousands of materials in the computer. And we were doing this specifically for improving the cathode material in a lithium-ion battery.

Anubhav Jain 05:39
So at the time that I started, a lot of people thought that this was infeasible. It would be too difficult to even just come up with the parameters that you should use for different materials. Each material might need slightly different settings for the calculation. So we had to come up with very custom rules about for this material use this sort of a setting for this other material uses other sort of a setting. And so some

people thought that that would not even be possible to do accurately, other people thought that the level of computing would be too much in order to run all these calculations, and just keeping track of all the calculations would be way too much of a mess. Today, the situation has changed completely after we demonstrated this other research groups demonstrated this nowadays, it's actually very commonplace going from one research group or five research groups doing this in the world. Now, there's probably dozens and dozens of research groups doing this sort of computational screening, and even industry is doing the sort of computational screening. Now, the other thing that's changed is machine learning, which basically didn't exist at all, when I started my Ph.D., at least in material science. And now it's very big field. We can talk more about that, too, if you like.

Sarah Webb 06:39
Yes, absolutely. That was actually where I was headed. Because it seems like machine learning has become so important and so central to this now. I'm interested both in how you use it and how maybe the evolution of machine learning has pushed your field forward.

Anubhav Jain 06:58
So in 2006, when I started my Ph.D., machine learning really was not on the map at all. And around 2011 or so is when I would say some people started to think about applying machine learning and what they call materials Informatics at that time to material science. And basically, at that time, it was just a handful of us. I remember I went to the first session of machine learning applied to material science at the Materials Research Society conference, the biggest materials conference. And it was a very small conference room with five or six of us in the room talking about machine learning applied to material science. And nowadays at the Materials Research Society conference, the two largest rooms are basically dedicated to machine learning. And there's like hundreds of researchers in these sessions. Ten years ago, both the data sets and also the methods were just not at a point where machine learning was practically useful for a lot of different things where you could get the type of accuracy you needed. So we didn't have datasets of materials and their properties that you could use to train a machine learning model to predict their properties. And we didn't have necessarily the right algorithms to be able to do those things accurately.

Anubhav Jain 08:01
What's changed over the last 10 years or so first of all, we've been able to create very large datasets for training more complicated machine learning algorithms. In particular, what I mentioned about using large computers to predict the properties of a lot of materials inside of the computer itself, that's really been going on for the last 10 years and has generated a lot of high-quality data about materials and what their predicted properties should be. And that can be used now to train machine learning algorithms to do the same task but with much less computer time. So these days, the new methods, the deep learning methods, the graph neural networks, things like that: One can actually train the machine learning model to do what we were doing with these very large calculations, but now in a fraction of the time. The other thing that's happening is that machine learning is being embedded more and more into the daily kind of tasks that people are doing in material science.

Anubhav Jain 08:52
So, for example, a common thing that people need to do is characterize the material. So they've made some chemical composition looks like a powder, let's say, and they need to shoot X rays at it and look at a spectrum of the X rays that come out the X ray diffraction pattern, and that will tell them what kind of powder they made. And the interpretation of the spectrum is typically largely a manual setting process where you have some reference spectra and you try and figure out what's going on. It's slow and different people can disagree about what's happening. So one of the ways that machine learning is just kind of inserting itself into standard material science test is by having algorithms that can actually take the spectra for you and start interpreting the characterization. And so this will be both very fast as

well as nonambiguous you know, it's the same result no matter how many times you run, it is becoming useful in a lot of different ways, just the standard tasks that everybody does all the time. It's also becoming useful for accelerating the pace at which we can make predictions about materials because instead of a calculation that might take 1000 CPU hours to run. So let's say it takes like a few days on your laptop, you can now run that same calculation through machine learning and a few seconds and get back on the result instantaneously and be able to try a whole bunch of other hypotheses of materials.

Sarah Webb 10:04
Can you give me an example or two or of, I guess we could call them success stories, or things that we've been able to develop on this, say, faster timeline than what you were describing?

Anubhav Jain 10:17
Yeah. So I would separate this into two phases. The first phase is from nothing to lab discovery. So it's been invented in the lab. And the second phase is from the lab discovery to actually like a product that you can buy. In terms of going through both of those phases. I actually only really know one example. And it's still taken quite a bit of time. So this was a project actually by my postdoc advisor and my Ph.D. advisor, Gerd Ceder and Kristin Persson. They were doing a consulting project back in the early 2000s, where they were first trying to scale these calculations and predict alkaline battery materials with these calculations. This was for an industry partner. Duracell. They predicted some materials. It took a long time for Duracell to do anything with it. But just very recently, I think you can buy a Duracell battery that uses some form of the calculation and the materials that they sent them.

Anubhav Jain 11:03
But this first phase of going from nothing into something that is actually working at the lab scale, there's been many examples of that. So I mentioned during my Ph.D. project that we were looking for new materials for lithium-ion batteries, these are cathode materials that have longer capacity for the battery, or faster charge and discharge rates. So we actually identified three or four different new compositions that would actually have very good properties for lithium-ion batteries and demonstrated in the lab that they had properties competitive with the current battery technologies. Those were a few of the initial successes to show that you could actually start to invent materials inside a computer and that you could actually realize them in the lab after predicting them. Since then, we've done other similar projects on thermoelectric materials. So this is for waste-heat energy conversion, here, we're looking for materials, if you have a heat gradient, so waste heat from industrial processes or something, you can convert that to electricity. And there's only certain chemical compositions that have this thermoelectric property evaluated by something called the figure of merit. So we were looking in the computer for materials that would have a very high figure of merit for thermoelectricity. And we found several materials that potentially had this property and were able to make them in the lab as well. They we've done similar things for water purification recently, where we've been looking for materials that can remediate nitrate in water streams, and an experimental partner was able to make those alloys and show them that they work pretty well. So there's now more and more examples of going from nothing to lab discovery. The procedure of going from lab discovery to an actual commercial product, though is—involves many more steps than just showing things are working in the lab. And that that procedure, I think, still needs a bit more work to get going.

Sarah Webb 12:43
Makes sense. There's so many factors that go into making a product that's cost effective and that a company wants to produce in mass scale. I also want to ask you about some of these other uses of machine learning. In your research, I had seen the paper where you're using machine learning to mine the literature to get material science insights. And as a visualization tool, it's a different kind of machine

learning algorithm that still supports the work that you do. Can you talk about that a bit, and maybe where the idea came from for doing that?

Anubhav Jain 13:13
This is a field that has really, really taken off in the last five years or so. I started right before the big increase-- everyone today is heard of ChatGPT and all other large language models that now exists when working with text data. But back when we started, ChatGPT didn't exist. And what we were interested in doing was taking the scientific knowledge that exists in material science and trying to put it into a structured and searchable format. So, for example, you can already search for papers using search engines like Google Scholar, but there were a lot of questions that you couldn't answer about materials from the search engine. So for example, if you had a particular material that you were targeting, and you wanted to know: Was this material ever made before and how? There is no easy search engine to give you that answer.

Anubhav Jain 13:57
The other problem that we had is let's say we were screening materials for a particular application, thermoelectric materials for waste-heat energy conversion, and we came up with a list of 100 candidate chemical compositions that might be good for this purpose. Some of those compositions would have been studied before, and we'd like to know about it. But it was very, very difficult to actually go through this list of 100 compositions, look at has anyone studied this before. And if so, was it a thermoelectric and exactly what figure of merit did it have if it were a thermoelectric? So what we wanted to do was to just take all this knowledge that really just existed in the form of papers that were published and try to transform that in a way that was much more accessible for researchers. The idea here is that there's a lot of research that we might be doing that someone did in the 1960s. We had a key piece of information from an experiment in 1970. But we just don't have access to that information. So how can we bring that access forward? So what we wanted to do was then use natural language processing algorithms. So these are machine learning algorithms that work with text and work with text in the way that people talk normally with all the messiness and grammar and things like that and to transform that into a more structured format, something that could be in a database that you could search and really work with. And the initial motivation was really just to make things easier for researchers. So again, I'm writing a review paper about thermoelectric materials, how to actually get the information really, really quickly.

Anubhav Jain 15:21
But we noticed when we were training these algorithms that they were maybe capable of doing more than what we initially set out to do. And we're still working on structuring data from the literature and trying to work with things that way. But we also found that these algorithms were maybe learning certain things about materials as they were being trained. In particular, we were trying to build this particular feature, which is given an application-- so I mentioned thermoelectrics. Give me a whole list of materials that that have been studied before for thermoelectric materials. And the way that we do that is that we use these algorithms to come up with a vector representation of words. So turning the word thermoelectric into a series of numbers that represent that word, and turning each of these chemical compositions into a similar vector of numbers that represent those chemical compositions. And then we were looking for which of the chemical compositions had a similar pattern of numbers to the word thermoelectric taking the dot product of them. And that would actually tell us which of these chemical compositions would have been studied for thermoelectrics in the past. So, again, this was a feature that would allow us to look at a whole bunch of chemical compositions and say, which are the ones that are most similar to the word thermoelectric and had been studied before. One of the postdocs in the group, his name is Vahe Tshitoyan, and he's now at Google. And what he noticed is that sometimes there were chemical compositions that had very similar patterns that were thermoelectric, but no one had ever studied them as a thermoelectric before.

Anubhav Jain 16:42
So normally, if you go down the list, you know, the things that look like they were thermoelectric, and the vector pattern of numbers are all thermoelectrics. And then every once in a while, you hit one that doesn't look like that. And I think a normal researcher would just say, Okay, there's like 5% error and this algorithm and call it a day, and it's 95% accurate, let's go with this feature. But I think he was very brave and saying that, okay, maybe there's more here. And we can interpret this 5% not as an error, but as a prediction that this algorithm is actually predicting that this material could be correlated with thermoelectrics. And so we came up with all these different ways of saying like, Okay, how could this be a prediction? Is that a correct prediction? And things like that and came up with ways to compare these predictions against calculations to do things like what if we made this prediction the year 2000? Would we have seen this material in the year 2010? So we came up with all these different ways of test these predictions, and it turned out to be relatively accurate. This was like another interesting result about we can actually use these machine learning algorithms to directly predict materials as well as structure information from the literature.

Sarah Webb 17:42
That's really interesting. I'd seen your recent paper looking at visualization. How does that work?

Anubhav Jain 17:47
So we use visualization in multiple forms. So there's visualization of the crystal structures, for example. And so materials are composed of atoms: chemical compositions, like lithium iron phosphate. So one lithium, one iron, one phosphorus, four oxygens, but then they're also arranged in spatial patterns. And so lithium might be surrounded by four oxygens, or six oxygens, or eight oxygens, and the phosphorus might be coordinated six-fold by oxygen as well. And there's these spatial patterns in which these atoms arranged, and the spatial patterns really affect the properties of this resulting material. And so being able to visualize these patterns and visualize the bonds and visualize the networking of bonds, and things can be very important to understanding the properties of the material. So there was a staff member in the Materials Project, which is a big initiative that I work on here at Berkeley Lab. And he took the initiative to come up with a new visualization package for visualizing these crystals. And that allows you to do a lot of things that you couldn't do with a typical crystal visualizations package; that's really been helpful for our work. It's been helpful for users of this resource called Materials Project, in order to determine the where are the bonding patterns? What are the coordination patterns that might lead to a certain property of a material?

Sarah Webb 18:59
Why don't you talk a little bit more about the Materials Project and what that is and what your role is within it?

Anubhav Jain 19:06
The Materials Project is an initiative that we started, while the roots go back all the way to, I would say, to this battery screening work that I mentioned, maybe further than that to this consulting project for Duracell that I mentioned as well. But in 2011, we formally launched the Materials Project. And what it is it's a public database of calculated materials properties. So I mentioned we're using the computers to calculate the properties of lots of different chemical compositions basically catalogue the properties of every material that we can and put them online for other researchers to use for whatever purpose they need to use them for. And the way that we're doing this is through calculating the properties of materials. So I mentioned earlier in our research, we were using supercomputers to run lots of different simulations on different chemical compositions and compiling a database of battery properties or thermoelectric properties or all sorts of different properties of materials. So instead of just doing that one research project and publishing the paper or coming up with some new compounds, we've been

trying to take all these calculations that we've done and put them online in a resource called the materials project. So this is a website that is publicly accessible at www.materialsproject.org. And now actually has about 400,000 registered users.

Anubhav Jain 20:21
So it grew way beyond our wildest dreams. We started in 2011. I think most of us thought that only a bunch of people doing materials theory might be interested in this resource: 10,000 people around the world, let's say. But as it grew, the experimentalist found a lot of value in these calculations that we were doing for planning out their experiments, or even to do things like help interpret spectra that we were calculating: our calculated spectra versus their experimental spectra, things like that. Industry now has gotten very interested in the Materials Project. So the audience has really grown quite a bit over time. So I started in Materials Project when we launched around 2011. And at that time, my role was largely running all the calculations, fixing all the bugs, answering all the user questions. So really, it was it was a hectic time. And it was very much like a startup culture I would say, around 2011, where there were only a few of us making this big resource. Nowadays, I have more of a high-level view. So I'm the associate director of the Materials Project. And it's a little bit like flying above the clouds, where you miss some of the weather that's going on day to day, but you see some of the overall direction and trying to guide our worship materials project be going next? Should we be leaning more towards the people that are using the materials project for training machine learning algorithms? Should we be doing more things that would involve the experimental community and these sorts of initiatives?

Sarah Webb 21:41
So I want to go back to this problem of new materials. What about synthesizing new materials? How does that process work for you? Is that something that you are involved in directly? Or do you collaborate very closely with people who do that?

Anubhav Jain 21:53
Traditionally, the synthesis part has been one of the more challenging parts of this whole coming up with something in the computer and then demonstrating it in the lab. When I was doing my Ph.D. work and we were looking at new battery materials, for example, we were coming up with lots of predictions in the computer, but we didn't have enough people in the lab. So our research group had both computer people as well as lab people. And we didn't have enough people in the lab to actually make all these predictions. So I just kind of volunteered to get trained in the lab and put on a lab coat even though I have no particular skill in synthesis, just because there was such a big bottleneck. It would often be two to three months of work to try and make one of these new materials. And that's if it could be made at all. So this sort of work is very difficult to do and very difficult to get people motivated to do because you never know how it's gonna turn out. And traditionally, we've either had to kind of do it ourselves within the same lab or find external collaborators that are willing to take a chance on some of these predicted materials and synthesize them.

Anubhav Jain 22:48
Nowadays, we're actually working at Lawrence Berkeley National Lab, on a new way to do this part of the process as well. And so this is an initiative called A-Lab. A stands for automated or AI or could stand for for a lot of bunch of things. And this is something that I'm collaborating with my old Ph.D. advisor on, Gerd Ceder, who's really starting up this lab, and then we did a lot of this high-throughput calculation work together as well. And this is a facility that has synthesis robots, it's all it's like fancy baking, you mix some powders together, you put them in a furnace, you heat them up, you maybe mix it up some more. Instead of having someone like me do this process, we actually have robots that dispense powders, weigh the powders, mix the powders. We have robotic arms that transfer the sample into furnaces and take them out of the furnaces. We have robotic arms that can actually do the X-ray diffraction characterization that I talked about, to put them into this diffractometer machine, get

the patterns out and use machine learning to interpret whether we made the thing that we want it or not. And then use things like active learning and iterative learning to determine what the next experiment should be based on the result.

Anubhav Jain 23:49
So if you got very close to the result that we wanted, but just not the correct purity, let's say maybe we try another experiment that's very similar to the experiment that we did before the recipe that we use. If you get something that's completely different then maybe we try something very different in terms of the synthesis recipe. So this has really accelerated the process by which we can do these sorts of synthesis experiments and bring materials from the computer prediction to lab realization. And to give you a sense of the current scale of a lab, in about two weeks or so we were able to do, let's say 600 experiments with a lab. Whereas if someone like me were doing experiments for two weeks straight, I could probably do, I don't know, 20 experiments, 30 experiments, depending on how we were batching them. So it really is a big, big accelerant. And the good thing is that if the experiment doesn't work out, we didn't really lose a ton of our researcher time. We really just lost the facility time. And it also encourages us to take greater risks and some of the things that we're trying to make as well. So I think this is the next phase in terms of trying to accelerate the entire pipeline going from all the way from the prediction to the commercialization.

Sarah Webb 24:56
This conversation is part of a series that we've been doing on the podcast about creativity in computing. And we've talked about all of these different ways that you apply machine learning the way that you're thinking about computing and material science and how to make these materials faster. I want to ask the big picture question of what creativity means to you.

Anubhav Jain 25:18
To me, creativity is going outside the standard or expected operating procedure. So for example, I mentioned that Vahe, who was the postdoc that was working on this natural language processing project, was looking at this data of materials that have this high that product, but the word thermoelectric, but weren't known as thermoelectrics. And to me, it's a creative stuff to not do the standard thing, which is to say that these are error points, and to actually dig deeper and to ask the question, like, is this maybe something more than that? Is this a prediction? The similarly this this idea that we need a library to visualize crystal structures? And how can we design a library that allows us to explore these crystal structures in a way that that is necessary, and in a way that's very powerful, that involves creativity as well, because you're going beyond what the current visualizers can do, and you want to see what sorts of things might be possible. So in this case, Matt Horton, who's now working at Microsoft, was the one that was doing that particular project. So I think anytime you're maybe thinking beyond what's the standard operating procedure from before, that is, you know, the creative part. And that's certainly the fun part of being in science. Because your whole goal is to go beyond what was done before, your goal is not to replicate the things that were previously done. Your goal is to figure out new ways to do things. And so it's certainly something where you get to exercise creativity very regularly.

Sarah Webb 26:46
And I want to ask you what advice you would give to other computational scientists, materials scientists who are coming up in this field? What do you like to pass along?

Anubhav Jain 26:58
I think one thing would be to not be afraid to take initiative to do things that are maybe outside, you're what you're supposed to be doing. So, for example, back when I was a graduate student or a postdoc, I felt that there were a lot of interesting things going on with machine learning and materials science, but

that nobody was really talking about it. And it was still a small field at that point back in 2011, or so. And so what I would really have wanted was for like Nature, to invite me to do a perspective on material science and machine learning. But I mean, I was a grad student or postdoc. so that was not really a possibility. So I just decided to start a blog on WordPress or something and call it Hacking Materials.com. The idea of hacking materials is using computers to hack how materials are made and things like that.

Anubhav Jain 27:43
And so I just started writing down my thoughts about machine learning in material science on this blog. But then it did start to get a little bit of traction, at least amongst the small community of people that were in the field. And it helped them if they didn't know who I was to actually know that there's this other person that exists that's thinking about these topics, having some fun with it, and things like that as well. So it was nice to kind of have my own platform for doing that. There's another professor at the University of Utah, his name is Taylor Sparks. And he's been doing YouTube videos about materials informatics, and he has a podcast called *Materialism* and about different material science topics. And I think that's great. And I wish more people would be taking the time to go kind of go off track a little bit and do what they think is needed, versus just the types of things that maybe they have to do there for their project.

Anubhav Jain 28:29
The other piece of advice that I might have is to – if there's a mentorship program – to maybe sign up for it. Even if you're unsure, and I was a part of a couple of mentorship programs here at LBL, where I was the mentee. And it really helped me understand the procedures at the national lab for things like promotions. How do I become a PI on a proposal? And what paperwork do I need to even fill out to be able to be PI on a proposal, a primary investigator and then give someone that gets funded on the proposal? These mentorship opportunities were very helpful for me to be able to ask these sorts of questions that maybe fill in the gaps of things that aren't always communicated in normal scientific conversation. And then if you later in your career actually sign up to be a mentor so that you can get to know people outside of the year research as well as to keep thinking about how research careers should go and give advice and pay back some of the stuff that you might have gotten as a mentee.

Anubhav Jain 29:22
So I think these programs sometimes are underutilized, and maybe they're underutilized by the people that need them the most, the people that are maybe too shy to sign up for them because they feel like well, I don't want to take up this person's time. I don't know what I would ask or things like that. But those are the people that might benefit the most from these sorts of mentorship programs. And if there is a program, then the mentor has signed up explicitly to try to help with these sorts of things. So do not be shy to sign up for these sorts of things. You know, the worst-case scenario is that you do it and a couple of hours of your time maybe didn't go the way that you wanted. And the best-case scenario is that you really understand better how to like get a promotion or how to move to the next stage in your career or really get a good new insight into the whole direction of your career. But the potential upside is really high, and the downside is very low.

Sarah Webb 30:06
I want to ask you a little bit more about the blog. I do think sometimes the traditional advice is "focus on your research." Can you talk a little bit more about, at least for you, what the benefits were of engaging with the scientific community in that way at that time?

Anubhav Jain 30:23
Yeah, first of all, I think it was just an outlet for me, where I had all these thoughts, and I just kind of wanted to get them out there somehow. So I think it was useful for me just to think through some of

these topics. Around the time that I was doing the blog, I was also putting in an application for a DOE Early Career Award. And these are awards that essentially propel you from being a more junior researcher to having your own research group and things like that. So it's a very important award, if you can get it. When I was doing the application for the awards, I was able to put down that in addition to all the publications and things. So I had this blog called Hackingmaterials.com. And I think it helps show to the people that are refereeing these proposals that this person is not just doing good research, but as a potential leader in the field. And so there are a lot of people I think, that have really good ideas, but don't necessarily have the resources to bring them to fruition. So being able to get those out and to show other researchers in the community what those thoughts are, I think can be very beneficial. The other thing is a time I was also doing this like hobby of learning how to draw and doodle and things like that. And the blog was a way for me to just add fun little illustrations to these materials, things. So it's, unfortunately, been a while since I've picked up that hobby again, but it was fun at the time.

Sarah Webb 31:33
Well, it seems like it was a nice way to bring a lot of interests together in one space, then.

Anubhav Jain 31:38
Yeah, exactly. And it was a lot of fun. When you do these sorts of things. I think it's important that you have fun with it, that it's something that you look forward to doing. Research can, at times, be filled with things that you don't want to do, whether it's like fixing a calculation that's failing, or whether it's like paperwork-type things. And having some kind of outlet that is very pure about the things that you're interested in, I think is just nice and refreshing.

Sarah Webb 32:02
Anubhav, thank you so much for your time. It's been such a pleasure talking with you.

Anubhav Jain 32:08
Yeah, it's been really nice chatting. Thanks so much.

Sarah Webb 32:10
To learn more about Anubhav Jain, the Materials Project and the Hacking Materials blog, check out our show notes at scienceinparallel.org. This concludes our creativity and computing series. If you're new to this series, you can check out the other three episodes on your favorite platform or on our website. If you'd like to support us, please rate the podcast and share your favorite episode with a friend or colleague.

Sarah Webb 32:38
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