

Science in Parallel Season1, Episode 6

Aurora Pribram-Jones: Building Big Science and the Whole Scientist

**SPEAKERS** Sarah Webb, Aurora Pribram-Jones

Aurora Pribram-Jones 00:00

People and projects in computational science

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#### Aurora Pribram-Jones 00:08

But you don't have to have role models, but it does change the landscape for you to change the possibilities of path that you see in front of you. It just gives you another example.

### Sarah Webb 00:17

You just heard from Aurora Pribram-Jones, Assistant Professor of Chemistry and Chemical Biology at the University of California Merced. Aurora is today's guest on <u>Science in Parallel</u>, a podcast about people and projects in computational science. And I'm your host, Sarah Webb.

#### Sarah Webb 00:37

In this first podcast season, we've been celebrating the 30th anniversary of the Department of Energy Computational Science Graduate Fellowship Program, commonly called C-S-G-F. Aurora was a CSGF recipient from 2011 to 2015, while completing a Ph.D. at the University of California, Irvine. They then did postdoctoral research at the University of California, Berkeley and at Lawrence Livermore National Laboratory. Join us for a conversation about unusual electron behavior, their nontraditional career path and the joys of teaching the next generation of scientists.

#### Sarah Webb 01:19

So, Aurora, welcome. This is going to be a lot of fun.

## Aurora Pribram-Jones 01:24

Thank you for having me. I'm excited to be here.

#### Sarah Webb 01:26

So I actually want to start and learn a bit about what research you're working on right now. What are you excited about?

### 01:33

My research focuses on what electrons do, especially when they're in weird situations, right? So you mentioned I came from some weird situation sort of, on my way to academia, and I deal with electrons that are also in, not bizarre, but different kinds of situations than the way we usually think about it. I'm a theoretical chemist, and most people who do that think about electrons that are in molecules or materials. And I do that, too. But those a lot of the time I'm working on developing like a mathematical toolbox to deal with electrons that are hot and dense at the same time. So they have thermal effects, like the effects of temperature, but they're dense enough that they still notice their neighbors. And so they still behave quantum mechanically. Other things that we work on are thinking about electrons, when you need a little bit more information than you have just in a single, low-energy state to describe what they're doing. So grabbing information out of the ether, that is the excited state and shoving it into the ground state in order to try to get a more accurate description of complicated electronic behavior. So I joke with kids — when I go talk at schools and things — that my job is to imagine things and draw pictures all day, which is really not very far from the truth. Like I act like it's me being cute, but it's not. It's pretty much what I do when I'm doing my research. And so we solve a lot of exact models, which are simple problems that we can solve exactly. So that we can really dig into them, and just put them through the business, right, like doing all kinds of crazy things, to models we know the exact answer for so that we can then extract that information and try to use it to build useful things for real-world situations.

### Sarah Webb 03:11

So what are some examples of some real-world situations where the things that you do are useful?

#### 03:18

So a lot of the work that I have is funded by the Department of Energy still because if electrons are hot and dense, they're probably in a few different places. You know, one of a few places one might be like in the centers of giant planets like Jupiter, in fusion experiments, particularly inertial confinement fusion experiments, where you're trying to move from this cool, chilly quantum state, and you squeeze things and radiate them, so that then they have to pass through the super complicated region of space that some people call the malfunction junction, that's really hard for us to figure out what's happening there. It's super complicated. And then you get to fusion and yay, fusion's been ignited. And you can use more of your plasma physics expertise. So folks who work in that, that malfunction junction is where I'm probably most useful, because it is really hard and complicated.

## Aurora Pribram-Jones 04:06

And so you can also find these things in other like astronomical events or just materials under extreme conditions. So if you slam stuff together really hard, that's another extreme condition that you might find, we have really high pressure is another area where some of my work might be interesting. But there are less big-sciency kinds of environments where my stuff might be useful. So you might find something like a system that has ground an excited state, so like, the lowest energy state, and then the state, that's just the next one up. Sometimes with electronic systems, like when we're just talking about molecules, it's a pretty big hop to get up to that first excited state. So you can't really do it again at room temperature very easily. But there are some systems where that's a lot lower, maybe your next excited state right, you hop up to the next rung of the ladder in energy. Maybe it's pretty easy to do that

because all you have to do is sort of wiggle your spin a little differently. You might be able to access a bunch of different kinds of states. And when you do that, you might need more information about what's happening outside of the absolute, the lowest-energy state. You might need a little information about what's happening in those, quote-unquote, excited states, because they're right there. Like they're very accessible. And so in those situations, right, when you might have something that's long and floppy, you know, a regular molecule might be interesting, even if it's not the middle of Jupiter or something. That's another area where having ways of dealing with not just the lowest energy state is useful.

## Sarah Webb 05:34

So everything from you know, what's right around us to the inside of Jupiter.

### Aurora Pribram-Jones 05:39

Yeah, a normal range of applications.

### Sarah Webb 05:45

So how did you get interested in this particular area of research?

### 05:50

In undergrad I, I transferred from community college to Harvey Mudd College, which is this like, tiny, wonderfully weird-slash-difficult place to be. It's a very small community, really intense. So you can imagine like coming in as somebody who's different was challenging, sometimes, like coming in as a transfer student was sometimes difficult, but it was a really rich experience for me. And while I was there, I got to do undergraduate research. I think I did it for three years, where I worked on liquid crystals. And I would synthesize this library of liquid crystals and look at how asymmetry changed how they blended together, how they mixed, so I got to sort of combine the synthetic chemistry with physical chemistry and then do some thermodynamic modeling. So thinking about how to model the energy components that went into how they were mixing.

## Aurora Pribram-Jones 06:38

And so when I went to grad school, I wasn't really sure if I wanted to keep doing experimental materials science or move more into the theory part of that work. And I ended up going to UC Irvine because there are a lot of really great theorists there. And, in particular, my PI in graduate school, my advisor there, Kieron Burke, set up like a separate interview for me, which let me meet more and more theorists. So when I started talking to him, he worked on density functional theory, which is the particular flavor of quantum mechanics that I work on. And I didn't come in thinking I would work on hot electrons, right? That wasn't, that wasn't a plan of any kind, necessarily. But when I was starting to apply for graduate fellowships, we connected with Mike Desjarlais at Sandia National Labs, and Frank Graziani, but in particular, Mike Desjarlais, who ended up being sort of another mentor for me. And he really helped us start this branch of Kieron's research group that is about thermal density functional theory. And so it was really exciting.

## Aurora Pribram-Jones 07:38

I got to sort of meet people who were working on this for the first time and building on work that had happened many decades ago, but was really starting to get play, because density functional theory

have been used at the national labs with great success in modeling these materials of extreme conditions that they were using things like the Z machine, and they were like density functional theory is working really well. Why is that? Isn't that not supposed to happen? Like, don't you need to have temperature in your theory to have it work? Well, I was like, Oh, that's a good question. Like, why, why is that working so well? I thought that was a really interesting problem. And the reality is that the CSGF is the reason why this is what I work on so much. We were working on it at that time. But my focus being in this area, was really due to me getting funding and getting to focus that way. And then getting to do a practicum at Sandia and connecting with people at Livermore, which is later where I did my postdoc. So all of those kinds of experiences and sort of having the bolstering that happens from like the alumni community and the practicums, and things like that, at the CSGF really focused my research in this area.

## Aurora Pribram-Jones 08:43

So I was excited, right? Like I mentioned, like extreme things are pretty exciting, it's a cool thing to do. If you can sort of step outside. I really do draw pictures on paper, like write equations on paper a lot. So to do work, that's on paper, but have it you know, be able to think about stars, or think about planets, right? Getting to think about astronomy, for you know, a weird pseudo-materials-science-condensed-matter-physicist-chemist, right? That was a weird and wonderful way to stretch outside of where I was, when you go to the national labs, I mean, big science is really intoxicating in a lot of ways. And so it was neat to be in a community of people who really deeply knew how these materials worked. They had huge insights, both experimentally, computationally and theoretically. But they're interested in my silly little model systems and like what I saw with these mathematical tools that I was working with, and that was a really fun way to see how my work could impact people working on real systems, which wasn't always as visible in other areas.

# Sarah Webb 09:50

But that's so cool. So tell me a little bit about density functional theory and what that is.

## 09:54

So density functional theory is a reformulation of quantum mechanics. So, you know, quantum mechanics is this special way of viewing the world, right? We're all quantum mechanical objects, and we're all classical objects. But it's this particular perspective on the world. And when you try to solve that problem for, say you have a bunch of electrons-- we use it for electrons a lot, because they're lightweight and fast enough that quantum mechanics really matters a lot for them. So if you want to solve chemical or materials science problems, you really need quantum mechanics. But it's devilishly hard to solve that for more than one electron at a time. I mean, you can solve it for two. You can get a lot of good answers for a small number of electrons, but for the number of electrons that you have, in molecule or material, it's impossible to do exactly, in practice. And so density functional theory is a way of rewriting that problem. So that you don't have to formally solve this coupled differential equation to get something called the wavefunction, right, which is describing the state that you're in, and it's this really complicated mathematical object. Density functional theory says: Well, what if instead of trying to figure out all these interacting electrons and what they're doing in the system that I care about, what if I instead had a system of noninteracting electrons, so I could deal with each of them separately? But I'm

going to put them into a different system that looks different, the landscape they live in is different. But that generates the same density. So the same probabilities of finding those electrons in those places.

### Sarah Webb 11:39

You mentioned that your path into science was not the typical road that most people talk about.

### Aurora Pribram-Jones 11:47

That's true.

### Sarah Webb 11:48

I guess I wanted to learn a little bit about what were the key steps that got you to science on this nontraditional path of yours.

### 11:56

My mom worked in scientific labs when she was a kid and things like that but shifted her focus to the rest of the world — things like being engaged in the community and making sure kids got fed and becoming a teacher and things like that. But it meant that our house was sort of run, sort of in between, like a mechanical laboratory and a biological laboratory and also a zoo. We had a lot of animals and things like that. My parents made it very clear — they had a lot of challenges that became our challenges as well. But one thing that I really treasure from their upbringing of my myself and my younger brother is that education and science were not confined to a place or a certain class of people. Our neighborhood kids were encouraged to come in and take all our books and read them and bring them back. And my mom was always asking us to do inquiry, right? Like that was how we were expected to engage with the world. And to think carefully.

## 12:56

And my family dealt a lot with incarceration. And the stories I heard about that from my dad were often about the books he was reading and things like that. So I grew up in a book home, and my dad was a mechanic. And so there were always engines opened up all over the place, and, you know, motorcycles, and you could go in there. And we had a lot of vehicles that were in many pieces and some even that ran. Science was happening all around me, even when I wasn't in school anymore. So I dropped out of high school when I was 15 because things had gotten very difficult at home and the world around us. Part of the fallout from that was that I didn't feel like I could be in school anymore.

## Aurora Pribram-Jones 13:35

And I started in community college, just because I wanted more flexibility. But I think that there was a period where I didn't think I was allowed to be a scientist in these places, like the places that I am now, because of leaving. And so it took me a while to allow myself to come back to science. And so I had a few different things that I did in the meantime. I was a music major for a while. I played the bassoon and sang and things like that. So I was a music major and did a bunch of other majors and had a lot of different jobs. And one of them was working at a bookstore called Stacy's bookstore that was a general and technical bookstore. And so once I was in charge, I had keys, and I could just sit in there and read at night or study. And so I started testing into science classes at the community college, but I think that was sort of the turning point for me, where I realized like, Oh, I keep reading all these science books,

and getting excited and like talking my employees' ears off about it, and they were very good natured about it.

## Aurora Pribram-Jones 13:38

But I am differently excited than even people who like science about science, and I and there's something that's driving me to read math and chemistry books, and want to take tests, right? Like that's a weird thing. Who wants that? That's bizarre, but like I really wanted to, I wanted to figure out how to do those things, and I really craved that, that formal education around those things. I really loved chemistry, but when I was in so when I tested into these classes, I ended up being a triple major in chemistry, biology and math. And working in tutoring centers there, like the math center there was mostly staffed by faculty, which was really great. I mean, I went to Foothill College in Los Altos Hills, which is a phenomenal community college. California's community colleges are astounding anyway, and it's a particularly strong example of that. And they trained me really well. They trained me really well in science, but they also trained me really well as a tutor. And as a peer mentor, and I was a part of programs there that really gave me an identity in science, like I was a science student. And I don't think that I would have gotten that otherwise.

### Aurora Pribram-Jones 15:49

And I had accepted the offer of admission as a transfer student as a biochemist at Berkeley when I got into Harvey Mudd, and I didn't really think that was going to happen. And so I actually sacrificed my deposit there, which was like a huge thing for me at that time of my life. I mean, I was not, I was like sleeping on people's floors at the time trying to balance all this stuff I was doing. And so you know, it's like \$200, or something, some exorbitant amount of money for me at that time. But I, I had a feeling that Harvey Mudd would offer me a different kind of opportunity because I was really worried about getting into somebody's lab as a transfer student.

#### Aurora Pribram-Jones 16:28

So I think a lot of my path was driven by the sort of diversity and depth of experience that I got to have living many lives before I went back to school. There are all these identity formation experiences that happened that I think really cemented for me that I was a scientist. And that was one of them: moving to Harvey Mudd, right, where, even if you're not a scientist, you're a scientist. You're a technical major or minor; that's how it goes. And it's way more about the experience of being in those classes and in those communities than what your major says on your transcript.

## Aurora Pribram-Jones 17:01

And then getting the CSGF, too. I think a lot of CSGFers have that moment where it's like, the deep imposter experience of your first program review when you go, and you're like, Oh, my, I should not be here, like these people are astounding. And then later, realizing that everyone is talking about that the same way, or at least a lot of people are, and realizing that you are part of this group and this community that further solidifies your role as a scientist and gives you a whole lot of pathways to pick from. I'm a deeply awkward person, but I'm strangely comfortable being myself or uncomfortable not being myself, I guess, is more appropriate, a better description of it. But I think that's because of having these like, really deep, super-strong formation experiences.

### Aurora Pribram-Jones 17:51

I worked at this Catholic seminary in the middle of that beforetimes. And so sometimes I talk a lot about formation, because that's how you talk about, like your calling, and your vocation and priesthood and stuff. I'm not Catholic, but I yeah, I played one for a while. I didn't. They called me heathen baby. And it was a really interesting experience. But I did that for a while. They're a big part of why I got to go back to school, actually, because they were so flexible about my schedule and things.

### Sarah Webb 18:18

But what's interesting now to me is that you are now in this role of professor, and you are now in the role of being that person, for students. And I guess I'm interested in what that's like for you now.

### Aurora Pribram-Jones 18:35

It's a huge part of my life. I really love my research. And, you know, being part of this research community and things like that, and I love mentoring my grad students and postdocs to my undergrads. But I the teaching part of it, though, I'm supposed to be in a classroom. It's like, I'm good at this stuff, but I'm really that's like where I'm supposed to be. Now I get to do that. And this exceptional community, right? I love being at UC Merced. Our students are astounding; they're brilliant. Most of our students are first-generation students. A huge number of them are dealing with things that I dealt with silently, or not so silently as you might imagine, sort of loudly and unconsciously, when I was an undergrad and grad student. And it's really powerful to watch them dealing with these things sort of in real time and to be able to be honest with them about who I am and where I'm from, and that where I'm from is not different now than when I was from there.

#### Aurora Pribram-Jones 19:40

But you don't have to have role models, but it does change the landscape for you. It changes what the possibilities of path that you see in front of you and just gives you another example. So I really like being able to do that for my students. I get to teach this honors introductory chemistry class, a General Chemistry 1 honors section, which is a very small class, less than 24 students. And it's their first chemistry class in college, almost all of them. So a lot of the times they're first-semester, and they've, some of them have never been on a college campus before. And they're talking to me about, you know, how do I talk to my parents about these crazy experiences that are so bizarre compared to what I was dealing with before? And I get to see these students that are meant to be doing science and are doing it despite a lot of messaging that they shouldn't be there.

#### Sarah Webb 20:26

Your website, I'm going to probably butcher hypugaea. Right?

## Aurora Pribram-Jones 20:30

That's right. I think that's right.

#### Sarah Webb 20:32

Is that right, the burrowing owl? I mean, your domain name is hypugaea. And, you know, there's this wonderful image you have of the burrowing owl and the support that you want to give to people who are

trying to emerge from the burrow. Right. And I mean, I look at a lot of scientists' websites, and it's just something that you don't, you don't see all the time, right?

## Aurora Pribram-Jones 20:57

Yeah, I represent a lot of different communities. And it's not always obvious. And so I didn't want people to have to guess, right, like going back to that thing, right? I want students to know that if they can see themselves in me that it's not an illusion. It's where I'm where I'm actually authentically from. And there's not a lot of room for that in those recruiting spaces or public. Like I don't know, I didn't know how to do that. So I actually really struggled with whether or not to put that. There's a certain page on my website that's about this sort of message to students and scientists. And you know, I've had people reach out to me on Twitter and, or through Twitter, about being gender nonconforming, and things like that, people who are not out. But saying like, it's really important to me.

### Aurora Pribram-Jones 21:40

Because I've thought about taking it down before, too, because I don't always-- People don't always react positively to it, right? But it is, it is distracting to some people because they're not used to people walking in the door with all that being visible. And I was very nervous putting it together. I have like vivid memories, trying to figure out how to do this in a way that felt true to me, right? Because I didn't want it to seem, I worry that it seems performative. And I still think about that sometimes. It is a big part of who I am and how I am. So I figured, better let students know, right? I'm probably going to ask about your mental health and your wellness all the time. And I'm probably going to be asking, you know, how have you engaged with your community today, right? Those things are important to me. And I think they're important to your science and your learning. And I think we don't think we do a disservice to all of us, when we, when we don't allow those tools to flourish, right? They really are cognitive, creative and analytical tools. And the more we keep people from acknowledging those things about themselves, the more we stunt their growth.

## Aurora Pribram-Jones 22:49

And so, yeah, it's my sort of blind and brute attempt to like, insert that into the scientific discourse just a little bit. Moving to UC Merced for me is like moving back home in a lot of ways. Not only in the fact that a lot of the students share a lot of the experiences that I had coming into academia, but also it looks kind of like where I grew up there, you know, these vernal pools, and there's a lot of marshy areas and they're these marsh birds all over: the red wing blackbirds and egrets and stuff all over the place. And that's a very deep part of my upbringing, like going out onto the bay lands and things like that outside of East Palo Alto, at the end of our street in East Palo Alto. And that was sort of where I felt safe and at home. And so when I was thinking about coming here, it's like, how do I tell folks that like, this is not a new place for me? This is a home place for me. And the owls were a big part of that for me because I remembered them there. And also they're super awesome and cute. They're like angsty, cute little birds. I don't know how you wouldn't like them. And they had these really long, spindly legs. If you guys haven't seen them, you should look them up. You know, I guess go to my website. Yeah, so it felt sort of gimmicky to name it something, right? So I struggled with this whole thing, but it really did start feeling more and more like myself and my students have really run with it. So, yeah, thank you. Thank you for bringing that up.

#### Sarah Webb 24:22

Can I ask you a few lightning round questions?

#### Aurora Pribram-Jones 24:24

Yeah, yeah, let's do it. I sometimes stumble on the lightning rounds. I'll try it. Let's do it.

**Sarah Webb** 24:30 Okay, as a chemist, do you have a favorite element?

#### Aurora Pribram-Jones 24:32

Oh, ah, do I have a favorite element? I don't know. I'm pretty into iron. I really like red earth, but this is the sounds dorky. Like it's not a good one. People are like really? Iron? Iron?? That's probably what it is. Because I think a lot about plants. Yeah, so I'm obsessed with plants. It doesn't look like that on my website. Looks like I'm obsessed with birds. But I'm obsessed with plants.

Sarah Webb 24:56

Oxidation state? You got a chem nerd for an interviewer.

**Aurora Pribram-Jones** 25:02 That's right. That's right. Oh, I don't know. Maybe four.

**Sarah Webb** 25:09 That's a nice round number.

#### Aurora Pribram-Jones 25:10

It is a nice round number. Okay, now I'm going to be thinking about that a lot.

Sarah Webb 25:19 Favorites subatomic particle might be easier because I think I might have a guess as to that one.

#### Aurora Pribram-Jones 25:24

Yeah, it is. I do love electrons. A lot. . . like a creepy amount.

#### Sarah Webb 25:35

And to wrap up, I want to ask you what, if you were to pass along one piece of scientific advice or life advice, or something that you would want early career scientists or young scientists depending on where they are and how they got into science, what would you want to tell them?

#### Aurora Pribram-Jones 25:56

I used to say that you should never choose by fear. And I think I stand by that still. Don't make your choices based on fear. I might have an addendum now that says like, make sure that they're, you know, girded with kindness, because I think that's hard for a lot of us. But I think they go hand in hand, right? I think if you choose out of fear, you're less likely to be kind because it's hard to be kind. Being

kind is bravery. Like that's a brave thing to do. You can be afraid-- just don't choose your path that way, like moment-to-moment or with the big goals. Do the scary thing sometimes, or maybe all the time.

### Sarah Webb 26:40

That's I mean that I mean, that seems like a great message to end on. No, I mean, not the easiest, but it's it seems like the wrap up.

**Sarah Webb** 26:53 Aurora I want to thank you. This was such a pleasure.

### Aurora Pribram-Jones 26:56

Thank you so much for doing this with me. I really enjoyed it. Yeah, anytime you want to go babble about electrons, let me know. Or owls.

**Sarah Webb** 27:07 I know how to find you.

Aurora Pribram-Jones 27:08 That's right. That's right.

### Sarah Webb 27:09

To learn more about Aurora and their work, check out the website hypugaea.com. That's H-Y-P-U-G-A-E-A dot-com. You can also find the link in our show notes at scienceinparallel.org. This episode concludes the first season of Science in Parallel, so please check out all six episodes. We'll be back in spring 2022, so please subscribe or follow us on Twitter so that you'll be in the loop. Science in Parallel is produced by the Krell Institute and highlights computational science, with a particular focus on work by fellows and alumni of the Department of Energy Computational Science Graduate Fellowship Program. Krell administers this program for the U.S. Department of Energy. Our music was written by Steve O'Reilly. This episode was produced and edited by me, Sarah Webb