Podcast Interview: Alán Aspuru-Guzik

PNAS: I’m Jessica Johnson. Welcome to Science Sessions.

The observable universe contains an estimated $10^{82}$ atoms. Now imagine atoms as LEGO® pieces that can be assembled in different ways to create new contraptions. The possibilities are nearly endless. Atoms similarly assemble to form molecules, and conservative estimates for the number of unique molecules that could potentially exist are on the order of $10^{60}$ to $10^{180}$. Alán Aspuru-Guzik uses principles of quantum chemistry to mine this vast chemical space for molecules that may prove useful in energy and electronics applications. Aspuru-Guzik is a professor of chemistry and chemical biology at Harvard University and has published in *PNAS* on a technique to investigate dynamic quantum systems using classical, rather than quantum, computing. I spoke with Aspuru-Guzik about his efforts to identify and build theoretical molecules for use in organic solar panels and batteries.

PNAS: Alán, one of the pieces of software that you’ve designed to identify potentially useful molecules for technological applications is named the “molecular space shuttle.” Why do you call it that?

Aspuru-Guzik: Imagine that you are sifting through all of the stars in the universe to find life. What we like to do is instead of going from one star to the other, we go from one molecule to the other, and we ask ourselves, “is this molecule useful or should we look into the next molecule?” So one of our softwares is called molecular space shuttle because we think about molecular space and we are using our space shuttle to explore it.

PNAS: The number of molecules that is known to exist naturally is a small fraction of the total number of theoretical molecules. Is there a way to determine whether a theoretical molecule built in the lab will be stable?

Aspuru-Guzik: The question of stability is the golden question. I have one new graduate student, her name is Jennifer Wei, that undertook the amazing project of trying to have automated tools to predict organic stability. And if we can tackle the stability problem, then all these material fields will benefit because if we have rules that tell me, just by looking at the molecule, with machine learning or with quantum chemistry, oh you’re gonna be stable, then I will look only at stable molecules and just throw away the unstable ones. So we already know a lot about quinone stability by data mining the literature of what happens to quinones and then now we know where are the
weak links in quinones, where are the places where a quinone will like to be reactive. So then if we know, then we can patch them so that the molecule is stronger.

**PNAS: One of the potential applications you’ve identified for the molecules that you are trying to build is in organic, metal-free flow batteries. What are the advantages of this type of battery over traditional battery technologies?**

**Aspuru-Guzik:** If you want to have a clean energy ecosystem, you need to have many components. It’s not only harvesting energy. You need to store energy temporarily. This is the battery space. Turns out that all battery technologies in the world, except a few exceptions, involve metals. We wondered if you were able to do all of this with just organics, which are known to be cheaper. That’s when we started looking at different alternatives and the quinones popped up as a good one. Ideally the battery that you want to have in your basement is something that if it spills, maybe it’s a little bit acidic but you can just mop it up. So what we do is we look at molecules that fall into the redox window of water. The quinones fall more or less in the right place. You have water, you add your quinone, you connect it to some wires, and there’s your battery.

**PNAS: You direct the Harvard Clean Energy Project. In this project, you essentially harness the computing power of PCs around the world to form a virtual supercomputer that calculates the properties of candidate molecules for organic solar cells. What are the advantages of organic over silicon solar cells?**

**Aspuru-Guzik:** We need them all. I imagine a future where we’ll have silicon solar cells, we’ll have nanoparticle solar cells, and we’ll have organic solar cells. Organic solar cells are very interesting for building integration because they are very lightweight. And therefore you could imagine having a solar cell stamp that you can put in a window that charges something. So I believe organic is going to have these niche applications that we don’t think about.

All of the processing of organic solar cells is made at room temperature and with liquids. You start with a roll of plastic that chemicals are being deposited onto and what comes out should be a packaged solar cell. The vision for these organic solar cells is going to be exporting to anywhere in the world a little press, like the newspaper presses, that is churning out the organic solar cells locally. And that I think is going to be the future.

**Me: What’s the current efficiency of organic solar cells?**

**Aspuru-Guzik:** It’s about 10% but it’s in the lab. Imagine those houses that you see around that have solar panels with 15% efficient silicon. I believe that you can get to 15%
organic as well. If organic solar cells reach some threshold parameters – I think it’s 10 years of lifetime, 10% efficiency, and $10 per kilogram—then they can be commercially viable and they can compete with silicon and they can find their niche applications.

**PNAS: How much success have you had in building these theoretical molecules for use in various technologies?**

**Aspuru-Guzik:** Many theoretical chemists have zero as a count of the molecules they have predicted and actually have made something. In 2007 I made a prediction that was actually done in 2011 for the first one. I call it my baby, it’s this organic electronics material. The second molecule that we predicted that was already successful was a flow battery anthraquinone disulfonate molecule. And that’s it!

**PNAS: Through the Clean Energy Project, you’ve released an open access database of theoretical molecules to the public. How many molecules are in the database?**

**Aspuru-Guzik:** 2.5 million, roughly. And I hope that my second generation of the Clean Energy Project, although I know many molecules from the first are being made right now, I’m pretty sure that the second generation will be much more useful. All the stuff that we’re computing is hopefully very easy to make so that what comes out from it is public domain information for anybody around the world to make solar cells.

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