ACS AMA: Hi Reddit! I am Kennie Merz, a professor of chemistry at Michigan State University. Ask me anything about computational chemistry/biology!

AmerChemSocietyAMA [1] and r/Science AMAs[1]

[1]Affiliation not available

April 17, 2023

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How will you Explain Protein Folding to a layman?

iaashish7

Great question and one that I faced at a high school class reunion a few years back! I was talking to an old high school buddy I hadn't seen for a few years ago and he asked, "So, what do you do" – classic high school reunion stuff – excitedly, I said, "theoretical and computational chemistry, where I use math and computers to understand biological and chemical systems – like drug design or protein folding". Whereupon my friend turns around and calls Joe over, "Hey Joe, come over here, you gotta hear this….". First you need to make sure that your audience knows what a protein is: Proteins consist of amino acid building blocks that form a 3-dimensional shape that then allows them to convert things like sugars to alcohol. Liberal use of your hands illustrating this seems to work well. Alcohol, as an example, works well too, since more often than not at a class reunion folks have had a few ;-). Once they get that you can tell them that the individual amino acids encode how the overall polymer folds up into its active 3-dimensional object – again liberal hand waving helps. That seemed to work for me, but perhaps my high school buddies were just being sympathetic to my condition – unrepentant geek!

As someone who worked in theoretical chemistry for a long while, are you concerned at all about how little mathematics chemistry majors are being encouraged to learn? I know that during my undergrad experience, I was one of the few physical chemistry students who went on to take PDEs and a handful of advanced calc courses because I was a math major as well.

When I got to graduate school, I was shocked at how little math my classmates knew and it definitely hindered a lot of them early on.

On a related note, how about the state of programming pedagogy? Scientists aren't exactly known for writing the cleanest code and following the best practices and as computers become more central in science, those weaknesses will become more dangerous.

TehMulbnief

See my comments on math above. Programming is another interesting problem. Early on there were too many operating systems (VAX/VMS/CMS/...), but we have now more-or-less focussed on a flavor

of unix to the benefit of the field. Early on if you were good at Fortran you were set, but now we have too many choices which causes confusion. Students code in Fortran, C++, python, java, etc. and coupling with tools like MatLab and Octave we have a mish-mash. I am not sure how to deal with this, but focussing on one language for high-performce computing would help and perhaps over time this will happen.

As a fellow computational biologist who also develops software (for metabolomics research in my case) I am curious why you chose to patent your software and sell it as a business instead of making it freely available to the scientific community.

I am a PhD student finishing up my first piece of novel software that is yet to be published. I would love to hear your perspective on going free and open source vs patented and commercialized.

wunderforce

We could discuss/debate this for literally hours. Personally I don't think there is one good answer and you should go with what works best for you. If you want to fully open source then great, if you don't then great - it takes all types to make the world go round. Talk to your friends and colleagues in your field and see what they think is the norm in your field and then decide from there. Decide what you want to achieve - gain academic visibility for your work (citations!) or make money off of your endeavors. Maybe you open source your work for academics and charge companies. So many variations LOL!

As a teacher I'm always interested in hearing the experts:

What do you know that you think kids should be taught in school? (K12)

What do you wish your school had prepared you for better in your field?

Micp

Personally, I think we should have kids take more math. Math is key to my field and to the future of the US. Hence, we need to step up to the plate and realize this is where we are. Rather than rote learning I wish that problem solving would of been taught more in K-12. Working on a problem that requires working your way through it and bringing in information from disparate fields make learning so much more fun and better reflects the real world. In the end we must take what we learn and apply it to solve problems!

There's a lot of concern over designer drugs and how to regulate them when commercial labs can produce new versions with only minor tweaks to a few functional groups. As someone who works on the design side, how would you propose regulating this type of innovation moving forward?

true_spokes

Take the opiate problem that has gotten a lot of press recently. The literature is full of derivatives of opium and a simple rule was formulated to make derivatives (the Morphine Rule); hence, folks looking to circumvent this class of controlled substance has a rich vein to mine. The initial hope was by increasing the potency of derivatives the addictive character of these compounds would go away - an outcome that did not happen. I guess, this is a long winded way for me to say I have no idea how to deal with this scourge besides regulating this class of compounds as best we can and to stay informed.

So more of a side note, nutritional studies are finally starting to focus on the impact of gut bacteria to our overall health, impacts on digestion, obesity, overall health. Basically humans are not just a single organism but more of a host to thousands of organisms that keep us functioning properly. Has any of this started to be a consideration in your work of medical design? I bring this up because one of the biggest threats to these colonies is the introduction of medicines (proton pump inhibitors, etc) so while they address the problem they are designed to, we are oblivious at times to their impact on synergistic bacteria.

Zetavu

Great question! I honestly, don't have a good answer for and this would be better handled by someone working on this topic. When designing a drug you typically focus on one target protein, but side-effects are hard to avoid that, for example, affects ones gut biome. Stay tuned this field will evolve in the coming years and a clearer picture will emerge,

Hi Professor,

Really appreciate you taking the time out of your day to educate us :)

I'd like to know what would you say are the most promising areas (both in terms of career growth and future discovery/contribution) that a biochem undergrad student should focus on heading toward?

Thank you!

Eroitachi

Great question ☺! What I preach to my graduate students is to be flexible. By getting a STEM degree you are becoming a world-class problem solver and, as we all know, the world needs problem solvers! For example, my students have grown into a number of different careers by being flexible. Some work for computer or internet companies, some work in pharm/biotech, some work at universities and some work in financial/insurance companies. In the end follow your heart and follow your nose. Do what you love and more often that not it will work out. Sometimes following the hot field can be good or bad – realize what is hot today might be cool tomorrow. When I entered grad school and decided to do theory/computation my classmates thought I was nuts and was headed to ruination. Five years later computational chemistry/biology took off and the rest is history.

Hi Dr Merz, and thank you for your time.

You say that your education is in chemistry and chemical biology, yet you work so closely with computers. I wonder, how did you manage to educate yourself on the computational side of the job? Was it just a great interest, or did you participate in additional formal education?

Cee-Jay

When I was growing up I was interested in STEM in general. My dad was a scientist and I'll never forget when he brought home and early TI pocket calculator. He also brought home a beautiful high-power microscope that his company was throwing away so I got first hand views of life in drops of water. It just went from there. That said my first love wasn't the computer, but I am glad I took programming classes and did what I could do to become decently proficient. I no longer program extensively largely because I have so much on my plate and just don't have the time, but I still can get around the computer as well as most anyone. Its kinda like riding a bike....

Are there any new developments you were sure youd never see when you started out?

magnotitore

The absolute amazing development of computing both raw compute power and storage. When I started out I thought this would of moved along much more slowly than it has.

Is it possible to get into your field without a degree in biology or chemistry?

smthamazing

Yes, it is, but you should be coming from a STEM field. I had one colleague who got his PhD in applied math and became an exceptional computational chemist! If you are passionate about the field then you will find a way to make it happen!

How has your job/capabilites changed since the explosion of personal computing, then the internet, then mobile computing?

riazrahman

Wow, where does one begin. The evolution in computing has simply been amazing on many fronts. As a grad student the lab of MJS Dewar was one of the best equipped in the world at the time with a VAX 11/780 mini supercomputer rated at ~.2Mflop! Semiempirical calculations of systems of 10s of carbon atoms were quite expensive, but you let things run for a day or two and that was the way it was. You spent the rest of the time writing and reading the literature. At the end of my graduate career I was able to run a couple jobs on a Cray 1 supercomputer (~100Mflop), which was ~500 times faster than the good old VAX. That was quite the epiphany for me and I realized that computational chemistry was off to the races. My laptop that I am typing on is many times faster than the 1980s machines. With GPUs and advanced CPUs the modeling studies we can do no are just amazing. Concomitant with improved computer performance - think about the advances in storage – just amazing as well – I have a laptop with 2TB of cheap storage while the whole lab in the 1980s had 100Mb or so of very expensive storage, which was huge for that time. Personally, while there is a need for very advanced hardware, I do think picking the right problems is key. In other words, don't depend on the computer to pick your problems – understand what you can do with computational tools and pick cool problems to tackle.

What do you find the most interesting aspect of your work ?

bnmhjkuiopl

The fact that it varies from day-to-day. Something new is always cropping up so its never a dull moment!