Hi everyone, my name is Yura \*scroll\*

and my project is about construction of surfaces of proteins. In the picture you can see the usual representation of a protein and surfaces built from it by tools I developed. This challenge is relevant because traditional molecular dynamics approach to docking is often too computationally expensive. And docking is quite important for many vital problems of humanity such as drug design or viral dynamics. So we suggest using only surfaces of proteins for their spatial alignment, which requires way less computational power than full molecular dynamic simulation. And here comes my project - there are currently no protein surfaces in WL, so I decided to implement them in a package which is now available for any of you to download and use. There are two kinds of surfaces - solvent accessible surface - on the left, and solvent excluded surface - on the right. You can come to my poster tomorrow and ask me what those are. \*scroll\*

By the way, speaking of pdb-proteins it’s hard to bypass protonation since usually pdb files we get from X-ray experiments lack hydrogens. But now there is a way to fix it - a function in my package. Seriously, go check it out. I’m saying it because I did it myself \*scroll\*

I’m currently working at EPFL on a project about protein docking and I’ve already done a few pictures for it in mathematica. And there are not only pictures on the way - if you go to my community post and look at what can be done from where we are now, you’ll see clear signs that just getting surfaces by themselves is only the beginning. So, I’ll be waiting for all of you tomorrow, thank you!