

Packmol - class test

Instruction: Create a single zip file, named with your group members, containing all packmol input files, and upload it on MS Teams.

1. Using Packmol, create a 3D model of YY palmitic acid molecules forming a monolayer on a 15Å radius sphere. Orient the molecules so their COOH groups face the sphere and their tails point outwards. Make sure the palmitic acid molecules are packed as dense as possible.
2. Using Packmol, create a single system containing four water spheres of different radii positioned above a graphene sheet.