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In-silico stress-strain measurements on beta-solenoid protein lattice[1] RACHEL BAARDA, DANIEL COX, University of California, Davis — Due to their large material strength and potential for functionalization, beta solenoid proteins show promise as building blocks in biomaterials applications such as two- and three- dimensional scaffolds. We have designed a two-dimensional hexagonal lattice by covalently linking a beta solenoid protein, spruce budworm antifreeze protein (SBAFP), to a viral protein (4NCV) with C3 symmetry. Although the properties of individual SBAFP segments have previously been studied, the composite properties of this lattice had not. We use the molecular dynamics tool Gromacs to strain the lattice by deforming the simulation cell and measure the resulting stress. Periodic boundary conditions allow us to simulate an infinite lattice; implicit solvent is used to remove the effects of fluid strain on the results. Stress is computed as twice the difference between the virial and the kinetic energy over the volume of the simulation cell. We evaluate stress-strain curves for the diagonal elements to extract the corresponding elastic modulus.

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