

U01 – Biomaterials: Predictive Design, Synthesis and Material Properties

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New integrated modelling and experimental approaches are needed to improve biomaterial design and functional outcomes. Scalable computational modelling tools are required to integrate with and guide the experimental design of polymers in order to generate new biomaterials with predictable functions; avoiding the more traditional trial and error approach. Toward this goal, we utilize mesoscopic simulations with a coarse-grained description of silk proteins as multiblock copolymers, synergistically integrated with genetic protein sequence bioengineering and bio-inspired shear-flow focusing processing, to systematically demonstrate how biological silk spinning and the resulting features can be understood, predicted, and optimized *in silico*. This approach has enabled us to elucidate key design features, such as molecular weight and the delicate balance between hydrophobic and hydrophilic domains towards the formation of robust silk protein biomaterials, including protein solubility, aggregate size, and polymer network connectivity. This integrated approach provides a path forward to generate well-defined functional protein biomaterials by exploring the sequence–structure–process–property relationship both *in silico* and experimentally. Furthermore, there are direct implications for these findings for materials generation in general, whether protein-based or synthetic polymer-based, with broad impact in the ability to predict material properties *de novo*.