Programming Complexity into Molecular Systems

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Over the past 3 – 4 years we have demonstrated the ability to predict and therefore design small peptides that are able to self-assemble.[1-3] Moreover, the ability to predict the characteristics of the self-assembled structure has allowed us to translate this understanding of the nanoscale assembly onto the macroscale of soft material properties. Until now, this work has focussed on the ability of a single peptide sequence to provide a structural basis for the formation of the soft materials. However, as this methodology has developed the desire to introduce functionality into these soft materials has led to the progression of this work into the field of complex systems, with multiple components interacting to provide both a desired structure and function to the resulting material.

This contribution will provide a number of examples of these new systems currently being studied, which have the potential to be transformative in a number of industries – including the food and cosmetics industries and areas such as drug delivery in the pharmaceutical industries. In all three of these examples, the computational led design of new systems can result in dramatic savings of both the time and cost of producing new systems with the desired properties.

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[2] G. G. Scott, P. J. McKnight, T. Tuttle, R. V. Ulijn, *Adv. Mater.* **28**, 1329 (2016)

[3] A. Lampel, S. McPhee, H-A. Park, G. G. Scott, S. Humagain, D. R. Hekstra, B Yoo, P. W. J. M. Frederix, T-D. Li, R. R. Abzalimov, S. G. Greenbaum, T. Tuttle, C. Hu, C. J. Bettinger, R. V. Ulijn, *Science* **356**, 1064 (2017)