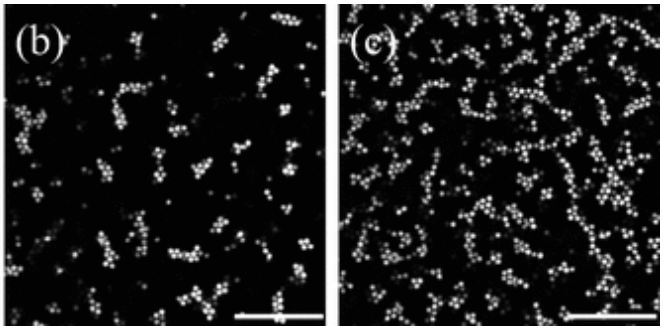
Digital self-assembly: learning to grow

About the project or challenge area: Equilibrium self-assembly is the spontaneous organization of molecules into a *single* new ordered structure – driven by a minimization of free energy. Biology does this with great precision and fidelity. Replicating a similar degree of control in the lab is probably the greatest unsolved challenge in materials chemistry. The problem is exemplified by *colloidal self-organization* of particles, which interact via a combination of short-range attractive (SRA) and long-range repulsive (LRR) forces. When these colloids are mixed together in solution, thermal motion generates a complex mixture of mutually competing phases – with portions of colloidal chains, helices, clusters, 2D rafts, and lamellar organizations all evident. Currently we have no theoretical framework to understand colloidal self-assembly and so cannot, in general, predict how to maximize the yield of any one of these structure or control assembly. As a result, industrial processes which depend on self-assembly of colloids require an empirical search of materials and protocols, which is time consuming and expensive.



We plan to use reinforcement learning to develop novel adaptive protocols for the control of colloidal self-assembly. Reinforcement learning is a branch of machine learning which is concerned with learning to perform actions so as to achieve a desired objective. It has been used recently to play computer games better than humans can. At Bristol, we have recently synthesized monodisperse colloids which interact via a SRR-LRR potential, which can be widely and precisely tuned. In earlier work, we have demonstrated that these particles can be assembled into colloidal analogs of polymer chains and clusters (see figure), using holographic optical tweezers to manipulate individual particles. We can "grow" colloidal polymers but the process is time consuming. We now wish to apply neural-network based evolutionary techniques to speed up and automate this assembly, using reinforcement learning to control our holographic optical tweezers system directly. Our aim is to produce a colloidal assembler which can be used to construct novel architectures, such as colloidal loops and knotted chains.

Why choose this opportunity? The focus of your project will be on developing sophisticated physical measurement techniques and demonstrating how they can be improved using machine learning methods. The project will provide an excellent platform to learn about AI techniques, digital microscopy, scientific computing, and the characterization of nanoscale materials and their practical applications. In addition to physical and computing skills, you will develop and increase your expertise in broad chemical synthesis and characterization techniques, whilst becoming familiar with the fundamentals of nanoscience. This project will require your collaboration with other members across other research groups, thus improving your teamwork and networking skills. Finally, you will be interacting with students from all over the world learning from their culture and skills, adding to your professional and personal development. You will be embedded in the Supervisor's research group, who will provide support. In addition, you will be assigned a mentor for the duration of your project, who will provide extra support and help you to identify any additional training needs or opportunities.

About you: You will have skills and knowledge in chemistry and a willingness to learn new skills in optics, microscopy and computation, where necessary. Full training will be provided.

Bench fees: A bench fee of £4000 is required.

How to apply: Applications are accepted throughout the year and you should complete the online application form for Chemistry (MSc by Research).

Supervisor: Your supervisor for this project will be Paul Bartlett, Professor of Soft Matter Science in the School of Chemistry. You can contact him at p.bartlett@bristol.ac.uk

Finding out more about your prospective research program:

Sherman, Z. M., Howard, M. P., Lindquist, B. A., Jadrich, R. B. & Truskett, T. M. Inverse methods for design of soft materials. *J. Chem. Phys.* **152**, 140902 (2020). 10.1063/1.5145177