School of Molecular Sciences
Arizona State University

# SMS 2023 P&T Seminar

## Thursday Aug 31 | 1pm | Biodesign Auditorium

**Multiscale modeling of nucleic acid nanotechnology and the quest for the holy grail of self-assembly**

The control over the self-assembly of complex structures is a long-standing challenge of material science, especially at the colloidal scale, as the desired assembly pathway is often kinetically derailed by the formation of competing alternative structures or amorphous aggregates. The goal of inverse design problem is hence to find a set of blocks that reliably assemble in high yield into a target structure while avoiding kinetic traps and alternative competing states. We present here a new design method, SAT -assembly, which solves this problem by mapping the design problem in terms of different building block types and interactions between them to Boolean Satisfiability problem (SAT). Using highly efficient algorithms developed for SAT, we can obtain solutions that can assemble into a target shape and at the same time cannot satisfy bonds in alternative competing states that have been previously identified in molecular dynamics simulations.

We then show examples of application of SAT-assembly design pipeline to several highly sought-after self-assembly designs: self-assembled Archimedean and finite-size polycube structures built from cube-shaped subunits. We use the SAT-assembly framework to scan the entire design space in terms of different numbers of building units, and compare the advantages and disadvantages of assembly kinetics of minimal designs (where as few distinct building blocks as possible are used) with fully addressable (each particle in the target design is unique species). We show that minimal designs, besides being more economical, often assemble better than the fully addressable ones. We use the SAT-assembly framework to design colloidal system that self-assemble 3D lattices that are of interest for optical metamaterial construction: pyrochlore and cubic diamond lattices. We successfully obtain solutions that avoid identified competing alternative structures (such as hexagonal diamond lattice) and successfully assemble in molecular dynamics simulations. Finally, we present a DNA nanostructure design pipeline, based on our coarse-grained model of DNA, called oxDNA, that can directly export abstract particle designs into realization with DNA origami. We show our preliminary results from experiments, where we have successfully assembled pyrochlore lattice out of building blocks designed and verified with coarse-grained simulations.


## Petr Sulc, PhD

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Petr Sulc is an Assistant Professor at Arizona State University. He received his bachelor's degree in Physics at Czech Technical University, Prague, in 2006, his masters in Quantum Physics at Ecole Polytechnique, Paris, in 2009, and his D.Phil. degree in Theoretical Physics at University of Oxford in 2014. He has worked as a research assistant at Center for Non-linear Studies in Los Alamos National labs and was an fellow in physics and biology at the Rockefeller University, New York. He established his lab at School of Molecular Sciences, Arizona State University, in January 2018. His research broadly encompasses applications of statistical physics and computational modeling to studies of DNA and RNA in biology and nanotechnology. He published over 55 publications in the fields of physics and chemistry. He is a recipient of NSF CAREER award in 2022.

*ZOOM option available: https://asu.zoom.us/j/84890997395