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Self-Assembly Method for Designing Lattices for Metamaterials

The ability to create nano- and meso-scopic structures with precise geometry is of immense interest and value in nanotechnology. Self-assembly with building blocks that encode the details of the structure is highly promising, but difficult to realize because of kinetic traps and unwanted byproducts. Although possible, it often requires painstaking trial-and-error procedures in order to get a high enough yield. With the development of advanced statistical mechanics approaches, it is possible to predict the self-assembly of complex lattices or finite size constructs. A common designing platform that targets multiple lattices while yielding solutions that avoid kinetic traps with assembly of only the target structure would be of great technological importance.

Researchers at Arizona State University and collaborators have developed a new modeling-driven design pipeline, using optimization methods and multi-scale simulations to design self-assembling DNA nanoparticles into a target structure. This modeling pipeline assures that the desired lattice structure is able to be created and at the same time that competing alternative states, previously identified in the simulation, cannot be formed. The model was tested by assembling a pyrochlore tetrastack lattice, both in silico and in the laboratory. While tested with tetrastack lattices, this method could be used for other lattices, multicomponent assemblies or even for designing initial seeding substructures or other sought-after lattice geometries such as clathrates.

This multiscale approach is able to design and verify in silico DNA nanoparticle that will assemble into multiple types of lattices or finite-size multicomponent assemblies using quick computational methodologies.

Potential Applications

- Sensing
- Photonics
- Imaging
- Energy conversion

- Waveguide manufacturing
- Optical computing

Benefits and Advantages

- Designs a desired nanostructure and assures that competing alternative states cannot be formed
- Can be used to form tetrastack lattices, which are highly sought, as well as other lattice-types
- Can be used to form finite-size multicomponent assemblies
- Can be coated and/or functionalized with DNA and positioned in 3D at nanometer precision
- Can realize metamaterial devices on UV or visible light spectrum
- Is able to verify mechanical stability in simulations and that the design is functional by self-assembling the nanostructure in solution and imaging with SEM

For more information about the inventor(s) and their research, please see

Dr. Sulc's laboratory webpage