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Case ID:M20-193L^
Published: 12/20/2020

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System to Design Self-Assembled Nanostructures with Patchy Particles

One of the fundamental goals of nanotechnology is to take advantage of the selective and directional interactions between molecules to design self-assembling structures with desired properties. The nanofabrication strategy by self-assembly has a main drawback that interactions between building blocks have to be designed to assemble target structure and avoid competing undesired assemblies. We present a method that models the assembly as patchy particles (PP) with interaction sites (which can correspond e.g. to colloids or DNA nanoparticles). Designing interactions between PP requires an efficient search in a large discrete space of possible patch interactions. The greater the possible number of interaction and particles types, the more computationally intensive it becomes to enumerate all possible patch assignments.

Researchers at The Biodesign Institute of Arizona State University and collaborators have developed a system to design self-assembled nanostructures from objects with geometric constraints e.g. PPs. This system provides a way to design interactions between these nanoparticles so that they assemble into the desired shape. This novel system provides, for the first time, a powerful method to formulate the self-assembly problem such that it can be solved within seconds to minutes to design extraordinary structures for chemical, physical and biological nanotechnology applications.

Potential Applications

- Could be used to construct optical metamaterials for information processing with light

o Chemical sensing, optoelectronics, quantum information processing, photovoltaics, semiconductor applications and more

- Smart drug delivery vehicles, self-assembled structures for medical diagnostics, semiconductor nanowires for flexible electronics, microspheres for opal optics and other biotechnology applications

Benefits and Advantages

- The algorithm allows the self-assembly problem to be solved within seconds to minutes

- Allows for specific target lattice, possible solutions and solution verification, where only the solutions that reliably assemble will be selected

- The method has been in silico verified to assemble into the pyrochlore, cubic diamond and clathrate lattices
- Transforms the inverse problem of self-assembly of colloidal crystals into a Boolean satisfiability problem for which solutions can be found numerically
- Solutions that correspond to competing structures can be eliminated
- Produces designs for which the target structure is an energy minimum

For more information about this opportunity, please see

Romano et al - Phys. Rev. Lett- 2020

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

Dr. Sulc's departmental webpage