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RESEARCH TEAM | **INVENTORS**

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CHEMICALS & NEW MATERIALS HEALTH & BIOMEDICAL

Systems and Methods for Designing Self-Assembled Nanostructures

ADVANCED MATERIALS - NANOMATERIALS | DRUG DESIGN & DELIVERY SYSTEMS | TISSUE ENGINEERING AND NEW **MATERIALS**

Method that transforms the self-assembly problem into a satisfability problem (SAT) which is much easier to be solved numerically. A particle design is produced that self-assemble into highly sought-after structures, such as the cubic diamond and other photonic structures.

Technical Features

The method consists of a general algorithm for the design of self-assembling systems (category of processes by which elementary components organize themselves into ordered structures) of irregular particles in any arbitrary structure, which includes the possibility of preventing the formation of alternative structures. The focus is on the design of particle systems with specific interactions expressed by sites (called patches) on the surface, in order to obtain spontaneous assembly in the desired structure. To introduce selectivity into the model, each patch is assigned a "color" which encodes its binding properties, and which can be experimentally achieved with patches based on DNA strands. To determine the relative concentrations of the species and the colors of the patches of each species, the problem is mapped into a boolean problem (SAT) of easy numerical resolution. In the known technique, the traditional approach is micro-patterning (e.g., lithography), which is more expensive and does not allow self-assembly in the entire volume of the sample.

Possible Applications

- Self-assembly of both crystalline and finite-sized structures;
- Healthcare applications: nanomaterials that aid tissue healing and capsids for drug delivery;
- DNA-nanotechnology sector, as DNA-mediated interactions are highly programmable.

Advantages

- Inherently parallel self-assembly (i.e., occurs throughout the sample volume);
- Economic method.







