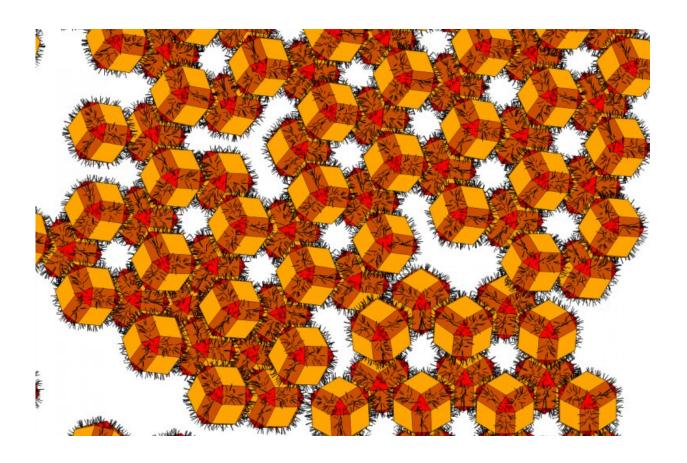


Formation of honeycomb nanostructures finally explained

April 29 2019, by Utrecht University



The simulation shows the honeycomb structure of the nanomaterial. Credit: Utrecht University

A few years ago, a promising new type of nanomaterial was observed experimentally, combining the virtues of semiconductors with those of



graphene. The material is formed by nanocrystals that spontaneously assemble into a honeycomb structure. Until now, it was unclear why the nanocrystals show this specific behaviour, but Utrecht researchers Giuseppe Soligno and Daniel Vanmaekelbergh have now developed a simulation model that reproduces the formation of these nanostructures in detail. The researchers published their results in *Physical Review X*.

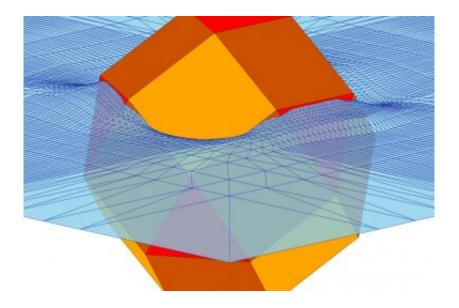
Optoelectronic properties

Square and honeycomb lattices are of great interest for semiconductor applications, thanks to their optoelectronic properties. "This unique combination of semiconductor nanocrystals that adopt the structure of graphene is one of the holy grails of materials science," Prof. Vanmaekelbergh explains. In their new model, the researchers have included all relevant forces involved in self-assembly. The resulting simulations show that tuning only a few parameters directs the final outcome. In particular, the assembled structure depends on the interplay between interface-adsorption forces and short-range electrostatic forces between the nanocrystals.

Controlled self-assembly

The model helps researchers understand how to experimentally control the self-assembly of the nanocrystals, and can easily be extended to study the self-assembly of nanoparticles at fluid-fluid interfaces into different structures. The results could eventually be used in the semiconductor industry to better produce nanomaterials.





A nanocrystal at the interface between two fluids. Credit: Utrecht University

More information: Giuseppe Soligno et al. Understanding the Formation of PbSe Honeycomb Superstructures by Dynamics Simulations, *Physical Review X* (2019). DOI: 10.1103/PhysRevX.9.021015

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