**Understanding the Formation of PbSe Honeycomb Superstructures by Dynamics Simulations**

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PbSe honeycomb superstructures, recently obtained by the self-assembly of PbSe nanocrystals (NCs) at fluid-fluid interfaces [1], have attracted a great interest since their predicted optoelectronic properties should combine the virtues of graphene with those of semiconductors [2]. However, their formation mechanism is still far from understood [3].

With a new coarse-grained molecular dynamics model we are able to reproduce the self-assembly of PbSe NCs in honeycomb and other observed 2D superstructures [4-5]. Our results shed light on the superstructure formation dynamics by identifying and quantifying the key parameters that drive the NC self-assembly into one or another superstructure. In particular, we show how the obtained NC superstructure depends on an intricate interplay between the interface-adsorption forces experienced by the NCs at the fluid-fluid interface and short-range electrostatic forces between the NCs. We also show indications that our model can be applied to study the formation and stability of defects in the self-assembled superstructures.

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