



FIG. 8 The morphology and structure of the CST/CS nanogel. The snapshot shows that there is more than one hydrophobic nanodomain in the nanogel structure. In addition, the complexation process was primarily driven through the hydrophobic interactions between the hydrophobic patch of FSH and the cholesterol groups of the hydrophobic nanodomains of the nanogel [64].

aggregates were formed onto the graphene sheets that were dependent on the water presence, quantity of lipid layers, and their initial orientations. Lipid layers were reoriented and self-organized to decrease the hydrophobic mismatches at the interfaces of water/lipid, lipid/lipid, and graphene/lipid. Several structures were formed such as inverted micelle-resembling assemblies, uniform layers, or weakly bound cylinder micelles over the monolayers that were approved by the experimental data. It was found that graphene could strongly order the lipid molecules directly contacted to its surface and located at 0.35- and 0.85-nm distances.

Graphene quantum dots (GQDs) exhibit exceptional mechanical and structural characteristics that make them valuable materials for application as drug carriers, bioimaging agents, and biosensors. Recently, MD simulations were carried out on protein HP35 villin headpiece that was adsorbed onto GQDs of diverse sizes [70]. It was displayed that the π - π stacking interactions among the GQDs and HP35 aromatic residues significantly affected the protein binding onto the GQDs. Also,

increasing the GQD size led to enhancement of the binding strength and number of adsorbed residues that increased the structural change by the adsorbed protein and this was confirmed through several protein structural analyses. Thus these simulations help to understand the GQDs biosafety and toxicity in designing biomedical devices based on GQDs.

4. CARBON NANOTUBES AND THEIR DERIVATIVES AS DRUG DELIVERY SYSTEMS

Carbon nanotubes (CNTs) and their derivatives such as boron nitride nanotubes (BNNTs) are interesting nanomaterials for application as drug carriers because they have high loading capacities and able to control the drug release rate [71]. Moreover, they indicate important and valuable physical and chemical characteristics. They are highly chemically stable and reveal compatibility with biomolecules such as proteins and nucleic acids and do not exhibit oxidative DNA destruction. The hollow tubular spaces existing in their structures lead to