Structure and Self-Assembly of Biomolecules through Molecular Simulations

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ABSTRACT

Recently, in the field of bio-inspired materials, the non-covalent self-assembly of relatively simple peptide based molecules has gained increasing attention for the formation of nanostructured, biologically functional materials, including nanofibers and hydrogels, all with nanoscale order. Moreover, polypeptide self-assembly is often associated with human medical disorders. Understanding the physicochemical determinants that underlie peptide self-assembly is a fundamental step, in view of the rational design, or redesign of already existed nano building blocks for biotechnological and biomedical applications.

Up to now our work concerns the modeling of small biological molecules, where the self-assembly propensity and the conformational properties, are studied through all-atom Molecular dynamics simulations using an explicit solvent model. A very common but of particular interest peptide, is diphenylalanine, FF. Our findings reveal a strong self-assembling propensity of FF in water in contrast to its behavior in methanol. We quantify the interaction between two isolated peptides dissolved in water/methanol through the calculation of a potential of mean force. Pair radial distribution functions between FF peptides, as well as the number of hydrogen bonds are calculated, providing measures of the self-assembly of peptides in the two solvents. Our results are in qualitative agreement with experimental observations.

Furthermore, the effect of graphene on the formed structures is examined. Atomistic details about the conformational preferences, the orientation of peptides with respect to the surface and the effect of concentration of graphene nanoparticles in water are presented. This detailed information provides useful insight into the mechanism of aggregate deconstruction due to the presence of graphene as well as, the way that peptides hinder the stacking among graphene flakes in water.

Finally, more complex systems, such as the Rop protein and its loopless mutation, RM6 have been simulated where, their structural, conformational properties, as well as their hydrogen bond network are characterized with atomic detail.

REFERENCES

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