

BN Nanosheet Induces Phase Transformation in Lipid Membranes

Jun Fan

Department of Materials Science and Engineering, City University of Hong Kong, China

Email: junfan@cityu.edu.hk

Boron nitride nanosheets are novel promising nanomaterials, which have a great potential in biomedical applications. However, there are very few reports about how they interact with the cell membrane. Here we employed large scale all-atom molecular dynamics simulations to study the interactions between boron nitride nanosheets and lipid membranes. Six different single component lipid membranes are examined. Our results reveal that the boron nitride nanosheet can extract phospholipids from the lipid bilayers and finally is enveloped by the membrane, which in turn affects the structural and mechanical properties of the bilayers. The bending moduli of the six bilayers all increase, while the diffusivity of individual lipid molecules all decreases. The corresponding molecular mechanism is that the acyl chains of local lipid molecules re-orient and become more ordered after the insertion of the boron nitride nanosheet. Particularly, the insertion of nanosheet induces a phase transition one of the bilayers. Our study provides novel insights into the biocompatibility of boron nitride nanosheets, which may facilitate the design of safer nano-carrier, antibiotics and other bio-nanotechnology applications.