

26th International Conference on **Advanced Nanotechnology**
&
2nd Edition of International Conference on
Materials Technology and Manufacturing Innovations

October 04-05, 2018 Moscow, Russia

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Mechanical properties and behaviors of low dimensional materials

With the rise of nanotechnology and the advances in interdisciplinary research, low dimensional materials (LDM) such as graphene have received intense global interest due to their unique physical and chemical properties over traditional materials. This talk is aimed to summarize our recent studies on the mechanical properties and behavior of LDM, including nanoparticles, graphene allotropies and two dimensional heterostructures, characterized using molecular dynamic simulations combining first principle calculation as well as theoretical analysis. Atomistic models of monolayer and multilayer graphene structures are constructed for the effect of surface functionalization (hydrogenation) as well as hybridization (with Boron Nitride) on the in-plane strength as well as thermal conductivity. Disclination theory is applied innovatively to the planar heterostructure with hybrid grains of graphene and hexagonal boron nitride for the key factors affecting the overall strength. Graphene multilayers with ordered interlayer characteristics are further constructed and analyzed. The coarse-grained MD simulations are performed to analyze the dynamic penetration process of LDM across a cell membrane. The evolutions of free energy as LDM piercing through the cell membrane are calculated by the innovative application of thermodynamic integration in nano-biological systems. The physical mechanisms of surface functionalization, stiffness and topological shapes on the penetrability of LDM are revealed by analyzing the change of penetration barrier and mode, and bioimaging experiments are carried out for verifications. Investigations about the principles and mechanisms of the mechanical properties and behavior of LDM are critical to its functional design and biological control.

Biography

Yinfeng Li received his Ph.D. degree from Shanghai Jiao Tong University in 2014, and now serves as an associate professor there. He has focused on the understanding of basic principles that control mechanical properties and behaviors of materials in both micro- and nano-scale. He has published 32 SCI indexed papers in high impact journals with more than 550 citations, including PNAS, JMPS, Carbon, Nanoscale, Acta Mater, etc. He has been selected in Shanghai Chenguang talent project and awarded the prestigious 'IAAM Scientist Medal' by International Association of Advanced Materials for notable and outstanding research in his field.

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