THE UNIVERSITY OF HONG KONG

DEPARTMENT OF MECHANICAL ENGINEERING

SEMINAR

Online

Title: **Physical mechanics of surfaces and interfaces in unconventional energy extraction and heterostructure/composite materials**

Speaker: **Dr. Kui LIN**
Postdoctoral Fellow
Department of Civil and Environmental Engineering
The Hong Kong Polytechnic University

Date: **16 August 2021 (Monday)**

Time: **11:00am**

Zoom meeting: **https://hku.zoom.us/j/98236923321?pwd=dDBKMjFySEhQazNxVjVHcFZ3MEtLZz09**
Meeting ID: 982 3692 3321
Password: 331127

Abstract:

At the micro/nano scales, the classical continuum mechanics cannot be applied directly and is modifiable by surface or interface terms. It keeps working when the surface or interface terms such as van der Waals (vdW) interactions are introduced. The physical mechanics properties of surfaces/interfaces in multi-phase materials will be presented. The main topics include adsorption/supercritical displacement of shale gas in nanopores (gas-solid interface), peeling mechanics of van der Waals heterogeneous structures (solid-solid interface), and debonding of fiber-reinforced polymer (FRP) composites (solid-solid interface).

Shale gas, consisting mainly of methane, is gaining importance as an unconventional energy source with abundant reserves. In order to investigate the adsorption/desorption and displacement mechanisms of the gas in nanopores, it is necessary to consider the atomic and molecular scale structure of the system from the perspective of quantum mechanics and statistical mechanics. Then, various experimental and molecular dynamic (MD) simulation approaches are combined to obtain a more fundamental understanding.

VdW heterostructures are designed at the atomic scale using layer-by-layer assembly of different 2D materials. The diversity of electronic structures of vdW heterostructures leads to the diversity of their functions. Although vdW heterostructures have promising applications, they are limited by the maturity of their structural assembly techniques. A bottom-up approach was used to investigate the exfoliation process of vdW heterostructures and a quasi-continuous method was developed to describe the evolution of the exfoliation force. Finally, a characteristic length was obtained, which is a key parameter reflecting the bending and interfacial properties of the laminate during the peeling process.

FRP composites, consisting of continuous fibres embedded in a polymeric matrix, have emerged as a durable construction material in the past three decades. A study on ReaxFF MD simulations of fibre-matrix interfaces in FRP composites, with a focus on the effect of fibre sizing, is presented. The sizing treatment was found to significantly increase the interface toughness while has little effect on the peak stress of fibre-matrix interface. The characteristics of the fracture surfaces and the scission of C-O bonds observed in the simulations are consistent with pervious experimental observations. The developed modelling method opens up a new avenue of investigating the deterioration mechanism of FRP under combined mechanical-chemical-thermal actions.

ALL INTERESTED ARE WECLOME
For further information, please contact Prof. AHC Shum at 3917 7904