Molecular Mechanics and Simulations of Organic Composite Materials

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Abstract: Organic composite materials can be readily found in our daily life, such as plywood used in construction industry and bamboo composites as indoor and outdoor flooring materials. These organic composite material systems consist of cellulose fibers bonded with each other through an adhesive, leading to a bonded system with a gradient structure that possesses a unique structural behavior, which has a great potential to be used as load-bearing building materials. In view of the manufacturing process of such composite material systems and the structure in-between the cellulose fibers and the adhesive, the interfacial adhesion of such systems at multi-scale would play a major role in determining their capability in load-bearing structural applications. In this seminar, the interaction between cellulose fibers and phenol-formaldehyde (adhesive) is chosen as a representative of the organic composite material system, and molecular dynamics simulation is used for quantifying the corresponding interfacial adhesion. The mechanism of such strong adhesion is a formation of hydrogen bonding between the cellulose and the adhesive. However, it is observed that the adhesion will be weakened in the presence of water, and hence the long performance and durability of such organic composite materials should be considered when such systems are present in civil infrastructures.

Biosketch: Dr. Denvid Lau is an assistant professor of civil engineering at the City University of Hong Kong. He obtained his Bachelor degree with first class honors and Master degree in Civil Engineering from the University of Hong Kong in 2004 and 2006 respectively, and received his Master of Science degree from the Department of Civil and Environmental Engineering (CEE) at Massachusetts Institute of Technology (MIT) in 2009. He then received his Ph.D. in the field of structures and materials from MIT in 2012. Prior to joining the City University of Hong Kong as an assistant professor in August 2012, he worked as a postdoctoral associate at MIT. Dr. Lau received various awards and scholarships including the Croucher Foundation Scholarship from Hong Kong and the Marvin E. Goody Award from MIT. He was named as one of the Harvey Fellows in 2011. His research focuses on the multi-scale modeling of organic-inorganic systems, wood mechanics, moisture-induced debonding, durability of concrete-epoxy systems and fiber-reinforced polymer (FRP) composites in structural rehabilitation.