Understanding the mesoscopic packing of calcium-silicate-hydrate through the unit building block concept

Dr. LAU, Denvid,
City University of Hong Kong

Abstract:

Atomistic simulations of cementitious material can enrich our understanding of structural and mechanical properties, whereas current computational capacities restrict the investigation length scale within 10 nm. This limitation prevents the consideration of many features of hydrated cements that originate at the mesoscale and are critical to macroscopic mechanical properties and failure modes. In this context, coarse-grained simulations can translate the information from nanoscale to mesoscale, thus bridge the multi-scale investigations. In this talk, the development a coarse-grained model of cement matrix using the concept of unit building block is presented. The objective is to introduce a new method to construct coarse-grained model of cement, which could contribute to the scale-bridging issue from nanoscale to mesoscale.