Department of Engineering Physics
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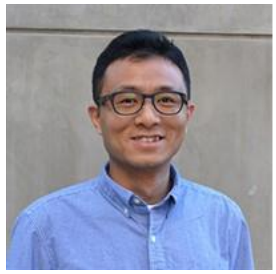

Presents:

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Structural Rigidity of Atomic Network During Irradiation-Induced Amorphization

Abstract: Concrete, a mixture formed by mixing cement, water, and fine and coarse aggregates is used in the construction of nuclear power plants, e.g., to construct the reactor cavity concrete that encases the reactor pressure vessel. Such concrete structures may be exposed to radiation (e.g., neutrons) emanating from the reactor core. To elucidate the concrete degradation in such environment, molecular dynamics simulations are conducted to investigate irradiation induced amorphization processes in the two major components of concrete, namely the mineral aggregates and cement paste. By characterizing atomic network topology within the framework of topological constrain theory, the resistance to amorphization under irradiation is found to be maximized in an isostatic atomic network. As such, the susceptibility to the mechanical and chemical degradation under irradiation can be quickly estimated for a wide range of silicate materials based on their atomic topology. Moreover, methodologies have also been established to evaluate critical mechanical properties, such as fracture toughness and creep modulus, of these engineering materials from molecular dynamics simulations.

***Biography*:** Bu Wang is an Assistant Professor of Civil and Environmental Engineering at UW-Madison. Prior to joining UW-Madison, he held an assistant project scientist appointment at UCLA. Bu Wang received his Ph.D. in Ceramics Engineering from Alfred University. He has broad research interests in applying atomistic simulation techniques to study mechanical behavior and physical-chemical processes of ordered and disorder materials.

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