A preliminary numerical study is carried out of the role on the bond behavior between silica and epoxy. This work is motivated by the experimental studies reported in [1, 2] wherein the interface fracture toughness of a fiber-reinforced polymer (FRP) bonded concrete system substantially decreases upon moisture ingress. However, a classical fracture mechanics-based approach at the meso-scale does not thoroughly explain this phenomenon and that the underlying deterioration mechanism in such a bi-layer system due to the presence of moisture remains largely unknown. Moisture-affected crack propagation in bi-layer systems is an intricate phenomenon that involves complex material evolution and chemical reaction mechanisms. Further investigation at a more fundamental scale is necessary to fully understand the mechanisms behind the observed behavior. This can be achieved by the use of molecular dynamics (MD) simulation. A silica-epoxy interface is chosen to be studied because these two materials have found broad applications in various structures in the construction industry, including retrofiting application of concrete structures using FRP. Silica is present in concrete in a large proportion as aggregate and usually constitutes more than 40 percent by weight of the solid ingredients in concrete production. In this paper, MD simulations of silica-epoxy interface with the use of the Consistent Valence Force Field (CVFF) are carried out under different temperature and moisture conditions. Two bonding parameters between silica and epoxy, namely the bond breaking energy ($E_b$) and the bond breaking distance ($\chi_b$), can be obtained by a Bell analysis [3]. Our method allows one to investigate the effect of moisture on mechanical properties of the interface from a fundamental, chemical perspective and may provide critical insight into the governing mechanisms of how moisture changes the fracture mechanisms of the interface.

References