Modeling fracture formation and propagation in cured epoxy resins under mechanical stress

Barışcan Arıcan[1], Christian Wick[1], and Ana-Sunčana Smith[1,2]

[1]PULS Group, Institute for Theoretical Physics, IZNF, FAU Erlangen-Nürnberg, 91058 Erlangen — [2]Group of Computational Life Sciences, Division of Physical Chemistry, Ruder Bošković Institute, 10000 Zagreb, Croatia

Epoxy resins, integral in manufacturing, play a crucial role due to their versatility. Understanding fracture mechanisms in these materials is paramount for determining mechanical properties. This study focuses on developing a multiscale simulation framework, integrating molecular dynamics (MD) with quantum mechanics/molecular mechanics (QM/MM), to consecutively assess and break bonds, simulating fracture propagation. MD simulations of straining crosslinked epoxy resin extend until the potential occurrence of fracture-inducing bond breakage, determined by bond elongation and referred to as the classical threshold. Subsequently, QM/MM calculations are performed on a small subsystem excised from the main system, precisely identifying actual fracture events through spin contamination assessment. Reaction site topology is then updated with broken bond information to create or propagate the fracture. Classical criteria triggering QM/MM calculations are optimized, ensuring computational resources focus on relevant fracture events. This work provides valuable insights into epoxy resin fracture behavior, advancing our understanding of these materials at the molecular level.