Uncovering the Chemo-Mechanics of Fracture via Quantum Mechanics Based Concurrent Multiscale Modeling

by

Derek H. Warner: Associate Professor, School of Civil and Environmental Engineering, Cornell University, Ithaca, NY 14853

Abstract: The prediction of crack growth is one of the most technologically important and scientifically intriguing problems in mechanics of materials. Yet, despite decades of research, a comprehensive understanding of the process has remained elusive. As a quintessential multiscale phenomenon, crack growth is both a chemical and mechanical process, involving interatomic bond breakage driven by long range mechanical stress fields. Thanks to growing supercomputing resources and novel concurrent multiscale modeling techniques that can accurately couple quantum and continuum mechanics modeling domains, crack tip processes in real environments are just now becoming accessible to powerful quantum chemistry approaches such as Kohn Sham Density Functional Theory. The majority of our work in this area has been focused on understanding how surface impurity elements influence the behavior of cracks in aluminum, a material that serves as the base of many technologically important alloys whose fracture response is known to be affected by chemical environment. In this talk, I will review our work on this topic and use it to frame our ongoing work.