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Multiscale modelling of fracture chemo-mechanics in brittle materials

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Modelling the catastrophic brittle failure of a crystalline silicon component, a rock specimen, or an advanced ceramic interface at the atomic scale is a challenging, intrinsically multiscale problem which requires a non-uniform-precision approach [1,2]. Failure generally occurs as a response to stress concentration, determined by the large scale geometry of the crack tip region, which alters the free energy landscape associated with the chemical processes occurring at the advancing crack tip. In turn, catastrophic or stress-corrosive bond-breaking events drive the dynamical evolution of the stress tensor field. The resulting chemo-mechanical coupling produces a rich variety of phenomena, such as fracture propagation instabilities[3], chemical fracturing induced by hydrogen segregation [4], and cleavage surface patterning [5].

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