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Quantifying the corrosive influence of water and carbon dioxide on crack propagation in silica

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The stimulation of crack growth in quartz and siliceous materials by hydraulic fluids or carbon dioxide (CO_2) injection remains an open issue when assessing the production of natural gas wells and long-term carbon storage. In this work, we employ reactive molecular dynamics (MD) simulations to study how the fluid environment (specifically, CO_2 or water) affects the mechanical properties of pre-cracked quartz grains. The thermodynamic conditions of interest are those relevant to subsurface reservoirs. Results from this study suggest that water and CO_2 substantially reduce the fracture toughness of quartz, thereby promoting crack growth and enhancing fluid transport in the subsurface. We report on how structural properties –bond length distribution and crack tip shape –evolve upon introduction of a fluid. These properties directly relate to macroscopic quantities of the global stress-strain curves, thus reaffirming the inherent coupling across multiple scales for fluid-solid interactions in the subsurface. Finally, the application of reactive MD simulations allows us to discuss the molecular processes that are causal for the observed chemo-mechanical processes at the continuum scale. The implications of this work may inform design principles for climate change mitigation technologies, including carbon sequestration, enhanced geothermal systems, and energy storage.

Time Block Preference

Time Block C (18:00-21:00 CET)

References

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