# Computing the dynamics of mineral dissolution and growth at the atomic-to-macroscopic scale in carbonate rocks

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Increasing computational capacities and availability of (sub-)nanometre-scale analytical techniques have led to new levels of understanding the complexity of mineral dissolution and growth. Among others, the role of mineral surface topography and the related structure of pore walls within Earth Materials is currently heavily investigated. A key question is how to upscale process- and rate-knowledge over many time and length scales?

In our current project, we will attempt to tackle this issue for carbonate rocks. Our approach hinges on a generally accepted assumption that calcium dehydration/rehydration is rate-limiting during calcite growth and dissolution in aquatic environments. Using molecular dynamics simulations, we investigated the impact of surface roughness, (non-)stoichiometry and impurities on water exchange kinetics of the calcium ions. A numerical model describing ion-by-ion growth and dissolution is (further) developed by implementing the variations in water exchange kinetics determined in our MD simulations. The numerical model is validated on microscopic and macroscopic experimental data and implemented in pore-network modelling. For more information on the projects see the abstracts of Janou Koskamp (atomic scale) and Priyanka Agrawal (pore-network scale).