Calcium carbonate – an “unwanted material”

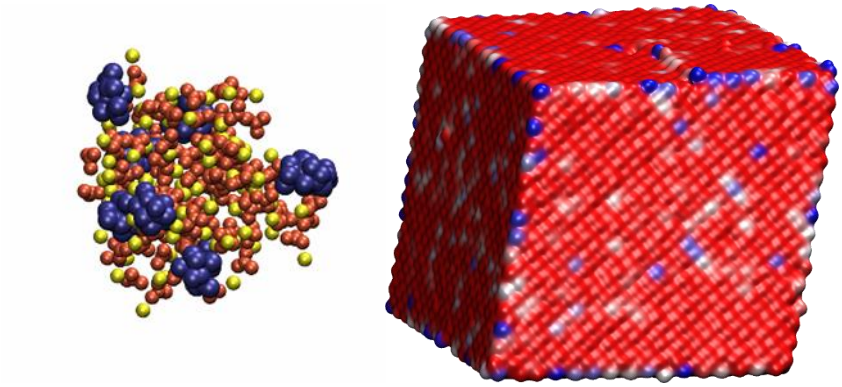
Patrick Duchstein[1], Stephan Wolf[2], Dirk Zahn[1]

[1]Computer Chemie Centrum, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91052 Erlangen, Germany

[2]Department of Materials Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Calcium carbonate, a ubiquitous material in nature, fulfills important structural functions for crustaceans, corals, mussels, and snails. In the household, however, it is largely undesirable. Kitchen cleaning agents, often working with alkaline pH values, unintentionally support calcite precipitation. Conversely, strongly acidic bathroom cleaners not only etch calcite, but also damage enameled surfaces. Despite its omnipresence and significance, our understanding of calcium carbonate structures in solution, calcite crystallization, and crystal dissolution remains rudimentary.

In this study, we present recent findings from investigating the interaction of precipitation-inhibiting additives with calcium carbonate in solution. Utilizing molecular dynamics simulations, we demonstrate how these small molecules dynamically interact with continuously evolving, entropically stabilized calcium carbonate networks in solution.[1] Furthermore, we construct a realistic model of a calcite nanoparticle, exhibiting a dislocation-induced continuous growth step. Our results illustrate how additives can effectively hinder further material deposition. Finally, we introduce a method for calculating instantaneous pK_a values specific to carbonate ions at the crystal surface and highlight the impact of acid-induced dissolution on the particle.[2]



[1] P. Duchstein, P. I. Schodder, S. Leupold, T. Q. N. Dao, S. Kababya, M. R. Cicconi, D. de Ligny, V. Pipich, D. Eike, A. Schmidt, D. Zahn, S. E. Wolf, *Angew. Chem. Int. Ed.*, **2022,** *61(40)*, e202208475

[2] P. Duchstein, F. Löffler, D. Zahn, *ChemPhysChem*, **2024,** *25(1)*, e202300489