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Insights into the metastability of amorphous calcium carbonate (ACC): Microfluidic experiments combined with an AI-assisted toolbox for quantifying mineral transformations

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Calcium carbonate is ubiquitous in both natural and anthropogenic environments. It occurs as various anhydrous crystalline phases, namely calcite, vaterite, and aragonite, as hydrated crystalline phases (monohydrocalcite and hexahydrocalcite (ikaite)), as well as amorphous (hydrous) calcium carbonate (ACC), with the latter being a potential precursor for the crystalline phases. The understanding of calcium carbonate mineral formation through ACC precursors is relevant for various systems such as biomineralization or the scavenging of metal contaminants and radionuclides. An artificial intelligence (AI) based toolbox was developed to process high-throughput data sets from droplet microfluidic experiments, automatically determining the time required for the transformation of ACC into crystalline phases and identifying the polymorphs formed based on their morphology. This proposed computer vision (CV) tool was developed by incorporating advanced image processing techniques and deep-learning CV methodology, whereby convolutional neural networks (CNN) incorporating the U-net architecture were used. This ensured a thorough analysis and classification of extensive datasets with a high degree of accuracy. The algorithm was trained and tested on droplet microfluidic experiments investigating the ACC transformation in absence and the presence of additives, i.e., Ba^{2+} ions. In the absence of additives, the half-life of ACC was evaluated at approximately 30 minutes with predominant recrystallization of ACC into vaterite. In contrast, in the presence of Ba^{2+} the stability of ACC was significantly increased with a half-life of about 12 hours and prevalent conversion into calcite. The developed workflow provides a robust and efficient toolbox that has the potential to significantly enhance the understanding and quantification of mineral transformations, providing also good statistics and reproducibility.