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New mechanistic insights for bacteria-mineral interactions learned from Kinetic Monte Carlo simulations

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Biological activity has the potential to alter or even completely change mineral dissolution or precipitation pathways. The presence of bacteria can inhibit or catalyze these processes and affect the chemical and physical properties of mineral surfaces. Bacterial colonization of mineral surfaces provides these microorganisms many benefits for using mineral substrates as sources of energy in the form of redox reactions, sources of nutrients, and as shelters from harsh external environments[1]. Bacteria-mineral-fluid system behavior is thus characterized by tight feedback loops between the organic and inorganic matter. The study of reaction mechanisms controlling material fluxes in this system is critical for understanding processes of bacteria-mediated dissolution and biomineral formation.

Schewanella oneidensis MR-1 is a common bacteria type that interacts with minerals and plays a critical role in the mineral dissolution process at natural conditions. Etch pits on mineral surfaces work as active sources of atomic steps, and thus act as active dissolution centers. Previous experimental studies revealed that Schewanella may substantially inhibit dissolution by attaching at etch pits, blocking the motion of stepwaves, and generating their own etch pits via metabolic activity[2].

The aim of this study is to understand complex feedback between bacteria and surfaces in the mineral dissolution process driven by etch pits. We utilize the Kinetic Monte Carlo (KMC) approach to simulate calcium carbonate dissolution in the presence of Schewanella MR-1. Preliminary KMC studies on Kossel crystals showed that this approach can be used as a heuristic tool for testing working hypothesis on bacterial influence[3]. Our current approach advances this idea further by incorporating realistic surface topography of calcium carbonate and making direct comparison to experimental data.

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