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Calcification of cell membranes: From ions to minerals

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Calcified microorganisms are a typical product of biomineralization. In this study, the whole process of cell membrane calcification of Bacillus licheniformis DB1-9 was studied by molecular dynamics (MD) and microbially-induced carbonate precipitation (MICP) laboratory experiments. Typical metabolitic products of Bacillus licheniformis DB1-9 were used as the calcium carbonate nucleation template to establish the organic constituents and a water-calcium carbonate two-phase system model for MD simulation, and to characterize the early stages of calcium carbonate nucleation on the surfaces of extracellular polymeric substances (EPS). The surface minerals of calcified bacteria obtained by MICP were prepared by focused ion-beam (FIB) and further analyzed using high-resolution transmission electron microscopy-selected area electron diffraction (HRTEM-SAED). We propose that the evolution process of cell membrane calcification is: ions → ion-pairs → multi-ion complexes (MIC) of large-size topological structures → pre-nucleated clusters (PNC) → amorphous calcium carbonate (ACC) → carbonate minerals (monohydrocalcite, vaterite, aragonite). In addition, ACC and the state before ACC were adsorbed on to the surface of the cell membrane after self-assembly in the aqueous solution; the ACC then underwent maturation and crystallized into ordered carbonate minerals with a crystal structure. Our study reveals the processes of microbial calcification, which has implications for the calcification of microorganisms in modern aqueous environments and for the formation of microbialites throughout the geological record.