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Inorganic precipitation mechanism of calcium carbonate polymorphs and their precursors

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Calcium carbonate, $CaCO_3$, occurs in six different forms: three crystalline polymorphs (calcite, aragonite, and vaterite), two hydrate phases, and amorphous calcium carbonate (ACC). These polymorphs are important both in life and material sciences, especially the occurrence of $CaCO_3$ in living organisms has received considerable attention. As a basis for understanding biomineralization, inorganic precipitation mechamism of these polymorphs has been extensively investigated for over a hundred years. Recently, crystallization pathway through non-classical mechanism such as stable prenucletaion cluster aggregation has been proposed, which give a new picture of the early stages of calcium carbonate growth. However our knowledge of formation process of $CaCO_3$, especially that of the mechanism of polymorph selection, is far from complete.

We have investigated experimentally and theoretically the metastable formation of $CaCO_3$ polymorphs and their precursors. In particular, the effect of Mg^{2+} on the nucleation and growth of $CaCO_3$ polymorphs has been focused and the quantum chemical calculations of Mg-containing $CaCO_3$ surfaces and clusters appearing in the early stages of $CaCO_3$ formation have been performed. As a result, Mg^{2+} substituted for Ca^{2+} affects the structure of surfaces and clusters, and may have significant effect on the polymorph selection of $CaCO_3$. In this presentation, we will report our results in detail based on the recent progress in this field.

Keywords: calcium carbonate, metastable phase, precursor