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Impurity effect for the formation mechanism of $CaCO_3$ polymorphs: ab initio study

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The formation process of calcium carbonate polymorphs has been extensively investigated because of its importance in both geological and biological environments. Recently, it has been pointed out that the surface energy difference among polymorphs could determine their stability field, so that it becomes more important to analyze in detail their surface structures and the incorporation process of atoms and molecules into the growth surfaces.

In the present study, first-principles calculation of aragonite (001) surface was performed to theoretically analyze its surface structure and growth process. Especially, here we focused on the case in which Mg^{2+} ion substitutes for Ca^{2+} site as an impurity. Because, different from Ca^{2+}, smaller Mg^{2+} is unstable in the nine-fold cation positions of aragonite, it can hardly incorporate into bulk aragonite crystal. However it is expected to be able to substitute for Ca^{2+} site in the surface bulk. Our simulation results show that Mg^{2+} can incorporate into Ca^{2+} sites in the surface with lower substitution energy than that for bulk, but Mg^{2+} on the aragonite surface considerably affects the surface structure. This suggests the possibility that Mg^{2+} could play an important role for aragonite formation and growth.

Keywords: aragonite, surface structure, first-principles calculation