Modeling of Carbonation and Neutralization Reaction for Reinforced Concrete

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ABSTRACT

Concrete, as a primary constituent of architectural structures, generally plays a crucial role in their durability and stability. One of its main reactions, the carbonation and neutralization reaction, is recognized for initiating the corrosion of metallic reinforcements, thereby influencing the long-term performance of the material. Nevertheless, it is still not easy to demonstrate the fundamental molecular mechanism underlying the reactions, owing to their complicated interplay with many factors.

Here we construct the theoretical modeling of the carbonation and neutralization reaction based on density functional theory to elucidate the underlying mechanisms of each reaction according to various factors such as humidity, acidity, presence of chlorides, etc. We calculate the transition states and reaction paths of the main reactions under different environmental conditions, with thermodynamic and structural properties. This study aims to unravel the key factors contributing to the degradation of the durability of concrete and also to offer a comprehensive understanding of their interrelationships. We hope that this research will facilitate the precise control of carbonation neutralization reaction in concrete, enhancing the durability of architectural structures, and finally making contributions to the concrete industry.