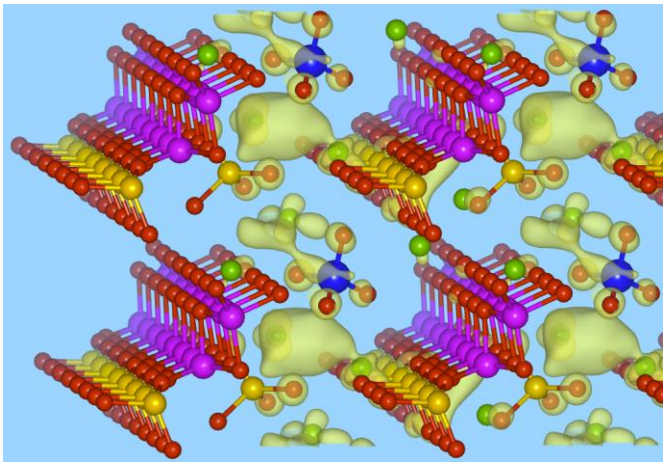
Aluminum and Sulfate Doped Belite

Problem

When compared with alite, a substantially lower manufacturing temperature and less limestone ($CaCO_3$) demand during production makes belite an ideal candidate for cement with a lower CO_2 footprint. However, its slow reactivity with water prevents belite-rich cement from fulfilling the required strength development standards and time constraints of construction, which dramatically reduces its use, and the more reactive alite phases dominate the make-up of cement today. A greater fundamental understanding of clinker phases, down to the scale of its electrons, is required to accelerate progress towards new generations of cement. Earlier we demonstrated the link between the reactivity profile of clinker phases and their electronic structure and also showed the possibility of engineering the dissolution and precipitation rates via the introduction of chemical impurities without losing novel elastic and mechanical properties.



Localized electron clouds (light yellow) in an aluminum and sulfate doped belite crystal obtained by quantum simulations. Green, orange, red, blue, pink spheres represent Ca, Si, O, S, and Al atoms, respectively.

Approach

In this work we employ first-principles computational modeling techniques based on a fully quantum mechanical analysis. Specifically, we show how the electronic structure of pure belite (C_2S) changes upon introducing different amounts of aluminum and sulfate into the system. We identify the most reactive regions by analyzing the charge localization in the belite crystal structure. By quantifying the charge localization factor, which determines the level of ionic character of the system, we predict how the reactivity of belite would be affected upon aluminum and sulfur doping.

Findings

The key finding of this research is that the ionic character of belite can be increased by introducing varying amount aluminum and sulfate into the system. The new formation of aluminum oxide chains together with the effect of sulfate ions localizes charge on or around the more ionic calcium atoms and thus creates new reactive regions. Such modification in electronic structure could significantly increase the reactivity of belite with water.

Impact

This research highlights the critical role of aluminum and sulfate doping on the reactivity of belite and indicates that by considering relatively simple chemical techniques, the dissolution and precipitation rates of belite can be significantly increased.

More

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