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Effects of $\mathrm{Ca}^{2+} \rightarrow \mathrm{Mg}^{2+}$ substitution on the properties of cementitious tobermorite

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ABSTRACT

AUTHORS

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- INTRODUCTION
- COMPUTATIONAL APPROACH
- RESULTS AND DISCUSSION
- CONCLUSIONS
- ACKNOWLEDGMENTS

SUPPLEMENTAL MATERIAL

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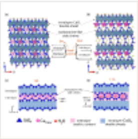
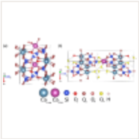
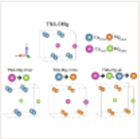
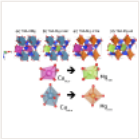
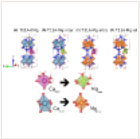
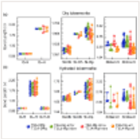
ABSTRACT

Using density-functional-theory calculations we assess the effects of the isovalent $\mathrm{Ca}^{2+} \rightarrow \mathrm{Mg}^{2+}$ substitutions on the mineral structure of tobermorite, a major analog of the main hydrated cement phase, calcium-silicate-hydrate (CSH). From the structural point of view, due to its smaller ionic radius, Mg substitution leads to an overall decrease of the lattice parameters for the 9 Å (dry) and 11 Å (hydrated) tobermorite structures used in the study. Furthermore, Mg doping at intralayer sites leads to a considerable distortion of the unit cell due to a changing oxygen coordination number. With the increasing amount of Mg doping, chemical bond analysis shows an overall increase in the bond strength with the crystal cohesion enhancement. In addition, Mg sites in the dry and hydrated tobermorite are characterized by an enhanced reactivity, which may be useful in capturing CO_2. With regard to the elastic properties, Mg doping leads to an overall stiffening of the elastic moduli. However, depending on the particular site, Mg doping may give rise to an increased elastic anisotropy. Overall, the present results indicate that Mg-based tobermorite structures may be useful prospects in the search for alternative components toward the development of high-performance, environmentally friendly cementitious materials.

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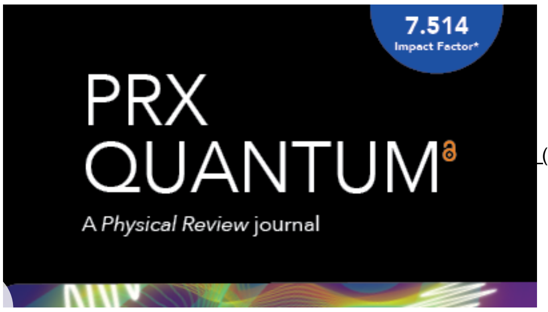

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