Atomistic Study of the incorporation effect of guest ions Mg^{2+}, Al^{3+} y Fe^{3+} in crystalline structures models of cementitious phases like alite (C_3S) and belite (C_2S)

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The presence of chemical substitutions is believed to play a crucial role in the hydration reactions, structure, and elastic properties of cement clinker phases. Hence, substitutions are of great technological interest, as more efficient production of cement clinkers would result in a reduction of CO_2 emissions, as well as possible economic benefits. Here we use a combination of classical and quantum mechanical simulation methods to study the detailed physicochemical changes of the clinker phases alite (Ca_3SiO_5) and belite (Ca_2SiO_4) when Mg^{2+}, Al^{3+} and Fe^{3+} guest ions are incorporated into their structure. Using classical force field methods [1], we considered random substitutions among possible sites and different compositions in order to identify the preferential substitution sites on the crystalline structures. Then, the resulting structural changes that take place to accommodate the guest ions are investigated and discussed in detail. Using quantum mechanical density functional theory calculations [2] the electronic structure of representative configurations has been computed to determine the potential impact of impurities on the reactivity.

[1] Tadmor, Ellad, B., Miller, Ronald, E., *Modeling Materials Continuum, Atomistic and Multiscale Techniques*, 288-298, Cambridge University Press, 2011.

[2] Jensen, F., *Introduction to Computationakl Chemistry*, second edition, 232-263, Wiley & Sons, 2007.