SILICATE CHAIN FORMATION IN THE NANOSTRUCTURE OF CEMENT-BASED MATERIALS

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ABSTRACT

Nano-scale processes in cement-based materials need to be understood in order to give rise to new tailor-made materials. Different experimental techniques reveal the presence of silicate chains of varying lengths in the nanostructure of cementitious materials. The length of these chains is crucial for the durability and performance of cement-based materials, and therefore the chain stability and forming mechanisms must be clarified. Here we report *ab initio* calculations on the stability of silicate chains and the pivotal role of certain ionic species on the chain forming mechanisms of the cement matrix nanostructure. Our results predict the empirically-observed magic numbers for the silicate chains, i.e. dimers and pentamers are the most stable species, and indicate that charged species are the most stable ones. Consequently, a colloidal description of the cement matrix nanostructure must be based on at least two basic units built from the most stable chains. The implications and the scope of our findings can be easily transferred to other similar systems and materials, such as clays, porous silicate materials, sol-gel materials, and more generally any silicate-based materials containing one-dimensional chains.