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Mechanism of molecular interaction of superplasticizer oligomers with hydrated cement phases

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Understanding the action of organic additives on hydrated cement phases is essential to develop novel admixtures and alternative cements with low carbon footprint. Due to the indirect nature of available experimental information the true nanoscale morphologies of the hydrated cement surface and its interaction with additives have remained elusive. Atomistic simulations with thoroughly validated PCFF-INTERFACE force field allow the first quantitative insight into the interactions of polyacrylate oligomers containing polyethylene side chains with tobermorite 14 A (h k l) surfaces in the aqueous solution. The results show that the acrylate backbone is more attracted to the surface than to the polyethylene oxide side chains. In particular, we found that carbonate ions of oligomers approach calcium ions on the tobermorite surface to form ion pairs. The adsorption energy on tobermorite facets per mole of acrylate monomer is in the range of 0~4 Kcal/mol. Detailed results for a range of different polymers and tobermorite facets will be reported and potential implications for hydration and setting properties will be discussed.

Biography

Tariq Jamil is a PhD student in University of Colorado Boulder, USA. He has completed M. Eng., from NED University of Engineering and Technology. Currently, he is working under Dr. Hendrik Heinz on the topic Molecularly designed construction materials.

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