

## Effect of Plasticizer Additives on the Mechanical Properties of Cement Composite: A Molecular Dynamics Analysis

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**Abstract :** Cementitious materials are an excellent example of a composite material with complex hierarchical features and random features that range from nanometer (nm) to millimeter (mm) scale. Multi-scale modeling of complex material systems requires starting from fundamental building blocks to capture the scale relevant features through associated computational models. In this paper, molecular dynamics (MD) modeling is employed to predict the effect of plasticizer additive on the mechanical properties of key hydrated cement constituent calcium-silicate-hydrate (CSH) at the molecular, nanometer scale level. Due to complexity, still unknown molecular configuration of CSH, a representative configuration widely accepted in the field of mineral Jennite is employed. The effectiveness of the Molecular Dynamics modeling to understand the predictive influence of material chemistry changes based on molecular/nanoscale models is demonstrated.

**Keywords :** cement composite, mechanical properties, molecular dynamics, plasticizer additives

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