# Molecular dynamics investigation of the effect of interlayer cavities of the structure of calcium silicate hydrate at the atomistic scale

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Calcium silicate hydrate (CSH) gel, as the most important component of hydration products, has the most significant effect on the properties of hardened cement paste [1, 2]. One of the most criticalfactors affecting the mechanical properties of CSHis the interlayer cavities in the gel [3]. In this study, the effect of these cavities on Young's modulus of CSHhasbeen investigated. For this purpose, first, the atomic structure of CSHis created, and then interlayer cavities with different dimensions are created inside the structure. For modeling, first, a super cell with dimensions of 3 × 6× 1 times the unit cell of Tobermorite is prepared, and then each of these layers areplaced on both sides of the new cell, and a space is created between these two layers. This distance is basically the cavity between the layers. The cavities are made in three sizes of 0.5, 1, and 2 nm, and water is then absorbed by the Grand Canonical Monte Carlo (GCMC) method. Then the created structures are simulated using the molecular dynamics method, and finally,Young's modulus is extracted. The results confirm the effect of the interlayer cavity on reducing the Young's modulus of CSH gel.As the dimensions of the cavity increase, the amount of water absorbed in the cavity increases, leading to a decrease in the Young's modulus of CSH.

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