

MOLECULAR DYNAMICS STUDY OF CALCIUM SILICATE HYDRATE ON POROUS SILICA

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The atomic structures of calcium silicate hydrate (CSH) in cement hold the key information of developing next-generation cementitious materials for civil engineering applications. Recent advances in determining the compositions and structures of cement hydrates have shed promising light on enriching fundamental understanding of CSH [1, 2]. In this work, the CSH molecular model is constructed by following previous determined structure in Ref. [2]. Quantum molecular dynamics simulations are performed to determine the structural stability of $(\text{CaO})_{1.65}(\text{SiO}_2)(\text{H}_2\text{O})_{1.75}$. Subsequently, large scale conventional molecular dynamics simulations with refined atomic force fields [3] are employed to study morphology of CSH on the surface of porous silica at various temperatures. It is found that CSH fills into the pores. Mechanical properties at the interface between CSH and silica under shear loading are investigated with different loading rates at various temperatures. Brittleness of cement is discussed from the view of water embedded in nano-scale layered calcium silicate hydrate.

REFERENCES

- [1] A.J. Allen, J.J. Thomas, H.M. Jennings, Composition and density of nanoscale calcium-silicate-hydrate in cement, *Nature Materials*, Vol. **6**, 311-316, 2007
- [2] R.J.M. Pellenq, A. Kushima, R. Shahsavari, K.J. van Vleet, M.J. Buehler, S. Yip, F.-J. Ulm, A realistic molecular model of cement hydrates, *Proceedings of National Academy of Science USA*, Vol. **106**, 16102–16107, 2009.

- [3] R.K. Mishra, R.J. Flatt, H. Heinz, Force Field for Tricalcium Silicate and Insight into Nanoscale Properties: Cleavage, Initial Hydration, and Adsorption of Organic Molecules, *The Journal of Physical Chemistry C*, Vol. **117**, 10417–10432, 2013.