

SILICATE CHAIN FORMATION DURING THE CEMENT HYDRATION PROCESS

A. Ayuela, D. Sánchez-Portal, A. Rubio and P.M. Etxenike

Donostia International Physics Center (DIPC), P.O.Box 1072, 20018 San Sebastian/Donostia. Spain

J. S. Dolado, I. Campillo, Y.R. de Miguel, E. Erkizia and A. Porro

Labein Centro Tecnológico, Cuesta de Olabeaga 16, E-48013, Bilbao, Spain

We have investigated by first-principle calculations the silicate chain growth and merging processes that occur during cement hydration. Our results suggest that the period of the empirically-derived equation $m = 3n - 1$ with $n = 1-2$ arises from the two pathways: Growth leading to dimers ($m = 2$) and merging to pentamers ($m = 5$).