Cement is a poorly crystalline structure, which is mainly built by C-S-H (CaO-SiO$_2$-H$_2$O) and a model of its formation includes a study of nucleation and growth of C-S-H nanoparticles. The first step in this investigation is to study the structure of cement-like materials, e.g. tobermorite 11Å. We used different kinds of tobermorite clusters: one represents a bulk (Ca$_4$Si$_{16}$O$_{46}$(OH)$_4$(H$_2$O)$_5$) and another represents a surface (Ca$_3$Si$_{11}$O$_{37}$(OH)$_3$(H$_2$O)) (Fig 1). Various types of embedding schemes were used: electrostatic potential, pseudoatoms, saturation by hydrogens. All calculations were made using Density Functional Theory (DFT/B3LYP).

Q: Where are water molecules inside the cluster?
A: The position of water molecule is determined by a possibility to create extra hydrogen bonds inside the structure. The position of water molecule inside the tobermorite structure was obtained by the set of single point calculations (Fig 2).

Q: What is the difference between isolated water and water in tobermorite structure?
A: The difference in the electronic structure between isolated water and water in the tobermorite can be seen on Fig 3. It shows that the electron density moves to the H$_2$O oxygen due to the ionic interaction with Ca. Therefore water in the tobermorite structure becomes more ionic. Moreover the influence of hydrogen bonds can be seen for oxygens which belong to SiO$_4$.

Q: How to build a cluster from periodic crystal?
A: The selection of clusters and surrounding point charges was performed by a new tool – ZYX script. The script uses a new ZYX format, which describes an arbitrary cluster by a sequence of commands defining the shape and the size of a crystal region.

Q: Which kind of embedding scheme to choose?
A: The embedding scheme which has been created by pseudoatoms with electrostatic field gives the smallest border effect in the cluster. In this kind of embedding the transition subsystem (pseudoatoms) creates termination region for covalent Si-O bonds. The comparison of Mulliken charges in various embedding schemes is given in Fig 4.

CONCLUSIONS

- Surrounding of the cluster by pseudoatoms with electrostatic field provides the best embedding.
- The interaction of water molecule with skeleton of tobermorite structure is relatively weak.
- The electron density of H$_2$O oxygen increases in tobermorite in comparison to isolated water molecule.

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