Structural, mechanical and vibrational properties of thaumasite from classical atomistic simulations

Tararushkin E.V.[1,@] **and Smirnov G.S.**[1]

[1] HSE University, Myasnitskaya 20, Moskva, 101000, Russia

[@] evgeny.tararushkin@yandex.ru

Thaumasite plays an important role in cement chemistry as the primary cause of sulfate corrosion in Portland cement at low temperatures of less then 15°C. This mineral forms a solid solution with ettringite which is usually present in cementitious materials [1].

The ClayFF force field [2] has been originally developed for atomistic computer simulations of clay and cement materials. We have shown recently that the ClayFF force field, modified by the explicit inclusion of Metal-O-H angular bending terms into the parametrization, (ClayFF-MOH, [3]), not only reproduces accurately the crystallographic unit cell parameters of ettringite but at the same time, noticeably improves reproduction of the elastic properties of ettingite and its vibrational properties. Here we use the same ClayFF-MOH force field to study thaumasite by classical molecular dynamics simulations.

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