The Hench Bioglass® 45S5 of 46.1% SiO₂, 26.9% CaO, 24.4% Na₂O and 2.6% P₂O₅ molar composition is of great interest in medical applications since in the presence of body fluids, and depending upon the rate of ion release and resorption, it creates chemical gradients which promote the formation of a layer of biologically active bone-like hydroxyapatite at the implantation interface. Osteoblasts can preferentially proliferate on the apatite layer, and differentiate to form new bone that binds strongly to the implant surface. Hydroxyapatite [HA, Ca₁₀(PO₄)₆(OH)₂] is the main constituent of the mineral phase in mammalian bones and teeth enamel. For this reason, HA is widely applied as an orthopaedic and dental biomaterial, both per se and together with other classes of materials, in the form of coating for metal alloys, in composites with polymers and so on.

In this seminar the quantum mechanical simulations carried out at B3LYP (within periodic boundary conditions as encoded in the CRYSTAL06 code) of both Hench bioglass and HA is reported. For bioglass, structure, electronic and vibrational features of the bulk are reported. For HA, bulk and main surfaces either free and when interacting with H₂O and glycine aminoacid will be addressed.