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High-pressure Crystallography, Weak Interactions and Electron Density. Andrzej Katrusiak. *Faculty of Chemistry, Adam Mickiewicz University, Poznań, Poland.*
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In 2009 the Crystallographic Community celebrates the half-century anniversary of the inception of the diamond-anvil cell (DAC) [1,2] – the ingenious, simple and low-cost device that triggered the structural studies in all high-pressure range from few MPa to hundreds of GPa, higher than at the centre of the Earth (364 GPa). Among several milestones in the development of the high-pressure crystallography were the introduction of gaskets allowing high-pressure studies at hydrostatic conditions [3], development of pressure calibration methods [4], common introduction of automatic diffractometers in the 1970's and 2-dimensional CCD detectors in the 1990's. These greatly facilitated high-pressure experiments. Now the DAC is commonly used for x-ray crystallography in many laboratories all over the world [5,6]. Furthermore, high-pressure is now well established in international and national synchrotron and neutron-source facilities, with numerous beam lines dedicated to high-pressure research.
The scope of high-pressure research is presently very broad, and includes the basic studies on very simple as well as complex systems for geology, physics, chemistry and biology, including several on-going projects on proteins and other biopolymers, and technological applications [6]. The quality of data recorded routinely in laboratories often allows the anisotropic refinements of non-H atoms and location of hydrogens from difference-Fourier maps in most cases, and accuracy of results comparable to those measured for bare crystals. High-pressures are ideal for investigating any structural transformations, as considerable compression of the crystal volume can be readily achieved in the DAC. This allows general description and understanding of thermodynamical processes, the intermolecular interactions and molecular electronic structure and their role for the molecular aggregation and crystal properties [7-9].

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Modelling of Biomaterials: Molecular Recognition at the Surfaces of Bioactive Glasses. Piero Ugliengo[a], Marta Corno[a], Albert Rimola[a]. [a]*Dipartimento di Chimica IFM and NIS, Torino University, Torino, Italy.*
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Among biomaterials, the Hench Bioglass® 45S5 of 46.1% SiO_2, 26.9% CaO, 24.4% Na_2O and 2.6% P_2O_5 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 re-sorption, 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 hydoxyapatite layer, and differentiate to form new bone that binds strongly to the implant surface. Hydroxyapatite [HA, $Ca_{10}(PO_4)_6(OH)_2$] 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 work quantum mechanical simulations carried out at B3LYP level within periodic boundary conditions as encoded in the CRYSTAL06 code to model bulk HA [1] and its main surfaces [2] as well as the Hench Bioglass® will be reported. For bioglass, structure, electronic and vibrational features of the bulk will be discussed [3]. For HA, structure and vibrational features of the bulk as well as the electrostatic features of the most important crystallographic surfaces will be discussed. For these latter, interaction with H_2O [4] and with five aminoacids (Gly, Ser, Lys, Gln and Glu) will be described in terms of most stable adsorbed structures and interaction energies. For the case of glycine [5] a detailed study of the role of co-adsorbed water will be addressed. The above results have allowed us to model the process of conformational stabilization of a short poly-glycine (12 residues) induced by the adsorption on the HA (001) surface as a function of mutations in the chain. This study is believed to be the first attempt to model by an ab-initio approach the interaction of biological relevant molecules with HA being the most important interface at the surface of bioglasses.

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KN-6

Phase Transitions in Nano- and Bulk-Materials at Elevated Pressures and Temperatures. Vladimir Dmitriev. *SNBL at ESRF, Grenoble, France.*
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Phase transitions induced by the variation of external parameters such as temperature, pressure, crystallite size,