

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Hydroxyapatite in Physiological Environment ALEXANDER SLEPKO, ALEXANDER A. DEMKOV, The University of Texas at Austin — A carbonated form of hydroxyapatite (HA) $[\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2]$ is one of the most abundant materials in mammal bone. It crystallizes within the spaces between tropocollagen protein chains in an aqueous solution and strengthens the bone tissue. An emerging application of synthetic HA is bone repair and replacement. Bulk electronic and chemical properties of HA were studied theoretically recently. However, the absorption of H_2O molecules and amino acids of the tropocollagen chains at HA surfaces remains an area of active research. Using density functional theory we analyze the electronic properties and surface energetics of HA for different orientations and terminations and generate a theoretical surface phase diagram of HA. The reactivity of these surface models is analyzed using the frontier orbital approach. We find two dominant surfaces which are most stable over the widest chemical range. However, we expect them to show little surface reactivity. Using a HA slab with a highly reactive surface we build atomistic models of HA covered with up to one monolayer of water and analyze interactions between this surface and the water molecules.

Alexander Slepko
The University of Texas at Austin

Date submitted: 19 Nov 2010

Electronic form version 1.4