

# Structural and electronic properties of $\beta$ Ti-based alloys by density functional theory

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The  $\beta$ -Ti-based alloys represent the second generation of biocompatible alloys that are suggested to be promising materials for replacing the widely used TiAl6V4 implants [1-2]. That is since the  $\beta$ -Ti-based metallic implants show lower Young moduli, higher corrosion resistance and minimal cytotoxicity. Nevertheless, in order to retain or improve these features and even include anti-bacteria properties further work is needed. This study consists of a systematic evaluation on the structural and electronic properties of the well known  $\beta$ -TiNb alloys in presence of biocompatible elements like Sn, In, Hf, Ga, Cu, Ag and Zr. Investigations on the ternary TiNbX (X= Sn, In, Ga) revealed that minor In or Sn additions (having sp valence electrons) introduce low energy states with s character that present antibonding features with the Ti first neighboring atoms as well as with the Ti-Nb second neighboring atoms thus weakening the chemical bonds and leading to elastic softening [2,3,4].

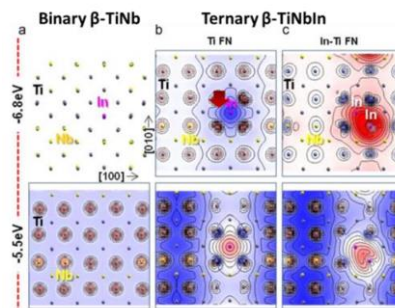


Figure 1: Electronic properties of  $\beta$ TiNbIn based alloys

On the contrary Hf substitution (sd valence electrons) in the orthorhombic Ti-Nb results in a phase transition to the  $\beta$ -phase due to Hf 5d contributions at the Fermi level and the Hf 6s hybridizations at low energies in the electronic density of states. Bonding-antibonding first neighbor features existing in the shifted plane destabilize the  $\beta$ -phase, especially at high Hf concentrations, while the covalent-like features in the first neighborhood stabilize the corresponding plane of the  $\beta$ -phase. New states close to the Fermi level are also introduced upon Cu substitution in the  $\beta$ -TiNb alloy. These results could be enlighten the design of  $\beta$ -type Ti-alloys suitable for metallic implants.

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