### Accepted Manuscript

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PII:	S0169-4332(14)01514-1
DOI:	http://dx.doi.org/doi:10.1016/j.apsusc.2014.06.193
Reference:	APSUSC 28245
To appear in:	APSUSC
Received date:	26-5-2014
Revised date:	30-6-2014
Accepted date:	30-6-2014

Please cite this article as: B. Wang, M. Lilja, T. Ma, J. Sörensen, H. Steckel, R. Ahuja, M. Stromme, Theoretical and experimental study of the incorporation of tobramycin and strontium- ions into hydroxyapatite by means of co-precipitation, *Applied Surface Science* (2014), http://dx.doi.org/10.1016/j.apsusc.2014.06.193

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## ACCEPTED MANUSCRIPT

# Theoretical and experimental study of the incorporation of tobramycin and strontium- ions into hydroxyapatite by means of co-precipitation

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#### Abstract:

Antibiotic incorporation into hydroxyapatite (HA) coatings by co-precipitation and the impact of bone relevant doping elements on the adsorption kinetics are investigated from both theoretical and experimental points of view.

Tobramycin interactions with bioactive  $TiO_2$  and HA surfaces are analyzed using density functional theory. According to the calculations, the drug molecule has larger adsorption energy than the Ca<sup>+</sup> ion on both surfaces under study in Phosphate Buffered Saline (PBS). The results support the experimental observations that HA nucleation and growth are strongly limited on  $TiO_2$  surfaces in the presence of clinically relevant antibiotic concentrations in PBS. The drug molecule is more likely to adopt parallel arrangement onto the HA surface, as the adsorption energy of such arrangement is higher compared to a perpendicular one. Strontium substitution of the HA surface is found to results in a weaker drug-surface interaction, and leads also to a decrease in coating thickness. However, the presence of strontium gives rise to a coating morphology with enhanced drug incorporation capacity and slower antibiotic release compared to non-substituted, co-precipitated counterparts. Our theoretical calculation results were found to be in excellent agreement with experimental data and provide a powerful tool to understand the interaction mechanism between drug and different surface chemistries necessary for development of future versatile orthopedic and dental implant surfaces. Download English Version:

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