

**W0281**

**Crystallographic, Electronic and Dynamical Properties of Pure and Silicon Doped Hydroxyapatite.**

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Hydroxyapatite and silicon doped calcium phosphates are now extensively used in the healing of human bone trauma. Silicon doped hydroxyapatite performs better than pure hydroxyapatite while a mixture of silicon doped calcium phosphates performs best. The recognition of silicon or silica as being key in bone remodeling applications has been established, but the mechanisms at play and even the material science and crystallography of silicon doped calcium phosphates, including hydroxyapatite, is still not well understood. The combination of theoretical *ab initio* and classical simulation methods in conjunction with experimental work has been our approach to investigate structural and dynamical properties of silicon doped calcium phosphates. We present the progress made in the theoretical calculations of electronic, crystallographic and dynamical properties of apatites and silicon doped hydroxyapatite and discuss the results in relation to our own experimental results and those of other groups.

Acknowledgements: Work supported by the NSERC of Canada, and Millenium Biologix Inc.