Structure-bioactivity relationships of phosphate-based glass from computer modelling

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Abstract

Phosphate-based glasses (PBG) have wide application as biomaterials because they dissolve when implanted into the body, with a composition-dependent dissolution rate that varies over several orders of magnitude. They can be synthesised containing different substances or materials, making them useful for controlled delivery of therapeutically relevant substances. In order to optimise PBGs for these applications, it is vital to understand the dependence of their dissolution rate on the glass composition and structure.
Over the past few years, computer modelling, typically molecular dynamics (MD) simulations, has pioneered our understanding of phosphate glass structure [1], particularly identifying the structural motifs which control the glass dissolution rate [2], such as the bonding of network modifying atoms to phosphate chains. MD simulations allow us to understand the ways in which therapeutic substances affect the glass structure and dissolution properties, which are often difficult to elucidate experimentally.

In this presentation, we outline results from our investigations into the structures of PBG doped with various cations, and the ways in which these cations affect the glass structure and dissolution properties. The ultimate aim is to be able to tailor the dissolution rate to a specific application and we will explain our progress toward this goal, making appropriate connections to experimental results.

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