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Enhanced Bioactivity of Nanosized Bioglasses: Computer Simulations

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Extended Abstract

Hench-type silica-based bioactive glasses such as 45S5 are used in biomedicine, for instance as bone defect fillers, in compact or particulate form. They also hold great potential for regenerative medicine, especially in their various nanosized forms such as nanoparticles (NPs) and nanorods, which have shown enhanced biological activity and antibacterial properties (Misra et al., 2008; Labbaf et al., 2011). However, in order to fully exploit this potential in practice, a better fundamental understanding of the origin of the superior properties of BG nanosystems is required: in this context, computer simulations are playing an increasingly important role (Tilocca, 2010; Berardo et al., 2014, Web-1). Recent Molecular Dynamics (MD) simulations show how the reduced size may affect structural and dynamical features in a BG nanoparticle of 6-nm size, in a way which could in turn enhance the bioreactivity of these systems (Tilocca, 2011). Here we present MD simulation data showing in detail how, compared to the corresponding bulk systems or to the NP core, reducing the NP size may lead to a reduction in the already low silicate connectivity of these materials, as well as to a higher Na^{+}/Ca^{2+} ratio and a higher mobility of Na cations, in the external regions of the nanoparticle directly exposed to the biological environment. We discuss several possible ways in which these nanosize-induced effects can give rise to - and thus be exploited to achieve - higher bioreactivity in BG nanoparticles.

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Web sites:

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