Molecular Dynamics models of a bioactive glass nanoparticle

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Bioactive glasses such as the 45S5 composition (BG45) are clinically employed as bone defect fillers in orthopaedic and dental applications. Their potential in regenerative medicine has also been highlighted but not exploited as yet, due to the lack of fundamental understanding of their composition-structure-activity relations. For instance, nanosized BG45 particles have shown enhanced biological activity and antibacterial properties, which could be the key towards developing a new generation of biomaterials for regenerative medicine. However, the rational development of these materials requires a better understanding of the origin of the superior properties of BG45 nanoparticles. Molecular dynamics simulations of a Bioglass spherical nanoparticle (approximately 6 nm diameter) have been carried out to investigate how the reduced size affect structural and dynamical features, which could enhance the bioreactivity of these systems. Compared to the bulk glass or to the 2D-flat surface of BG45, the simulations reveal that the reduced size leads to a further slight reduction in the already low silicate connectivity on the nanoparticle surface, to a ring size distribution shifted towards three-membered rings, and to a higher Na^{+}/Ca^{2+} ratio in close proximity of the surface. A higher mobility of Na cations in the external regions of the nanoparticle has also been detected. The possible ways in which these effects can translate into higher bioreactivity of BG45 nanoparticles are discussed.