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Developing Iron Oxide Nanoparticle Biosensors through Simulation and Modelling

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Abstract content
   (Max 300 words)
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It is well known that iron oxide nanoparticles exhibit magnetic and superparamagnetic properties at small sizes. These properties in magnetite in particular (Fe3O4) has been exploited for various applications ranging from memory storage and cell separation to theranostics including hyperthermia treatment of tumorous cancer cells, contrast agent in magnetic resonance imaging, cellular imaging and drug carrier in targeted drug delivery system. Forced oscillation of spherical iron oxide magnetic nanoparticles (MNPs) via low-power and low-frequency alternating magnetic field (AMF) is currently being used to kill cancer cells in vitro.
Small iron oxide nanoparticles may also possess a small amount of uncapped charge, whereas the positive charge on bare nanoparticles may be carefully engineered to suit a particular application. This leads to nanoparticles behaving as imperfect point charges and even dipoles in an external electric field. In this study it will be shown how these properties may be exploited to develop chemical and biological sensors. In particular molecules with a carboxyl functional group and hydroxyls are presented as case studies.
Designing such a system through experimental trial-and-error methods alone will be quit daunting without any prior knowledge of how such a system might behave under variable nanoparticle sizes and shapes, nanoparticle capping ratios, electric-field strengths and directions as well as electric field oscillating frequencies. Therefore modelling and simulation techniques prove very useful in tailoring this system.

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