Designing Gold Nanoparticles for Biomedical Applications: Insights from Theoretical Simulations

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Biomolecules adsorb differently to nano-structured materials and this phenomenon is being now widely exploited for engineering novel materials and devices for biomedical applications. At the same time, there is little knowledge of how engineered nanomaterials interfere with the overall biological molecular machinery [1]. Theoretical modelling can help get insights into the molecular mechanisms of biomolecular interactions of nanomaterials which can help improve molecular recognition needed for safe and efficient biomedical applications. However, some serious challenges exist in developing an adequate approach to modelling nano-bio systems with rigor and efficiency [2]. In this talk examples of our recent simulations performed in conjunction with experimental studies will be presented. These include: (1) effects of nano-structuring on protein adsorption to monolayer protected Au nanoparticles [3, 4]; (2) effects of peptide surface density on the efficiency of TAT peptide functionalised Au nanoparticles for membrane internalisation [5]; (3) effects of structure and dynamics of the functional peptide layer on the efficiency of epitope conjugated Au nanoparticles for biosensing [6].

References

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