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Gold nanoparticles in model biological membranes: a computational perspective

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Abstract

The electronic, optical, catalytic, and magnetic properties of metal nanoparticles (NPs) make them extremely interesting for biomedical applications. In this rapidly moving field, monolayer-protected gold nanoparticles emerge both as a reference system and as promising candidates for drug and gene delivery, photothermal treatment, and imaging applications. Despite the technological relevance, there is still poor understanding of the molecular processes driving the interactions of metal nanoparticles with cells, and with cell membranes in particular. In this paper we review molecular-level computational studies of the interaction between monolayer-protected gold NPs and model lipid membranes. Our review comprises a brief description of the most relevant experimental results in this field and of the questions they raised, followed by a description of the computational achievements reported so far.

1. Introduction

The electronic, optical, catalytic, and magnetic properties of metal nanoparticles (NPs) make them extremely interesting for a variety of biomedical applications. Metal NPs have unique optical properties: they exhibit a strong localized surface plasmon resonance[1] (LSPR) that can be exploited for both imaging (e.g. cancer imaging[2,3]) and near-infrared photothermal therapies[2,4–6]. The magnetic properties of metal and metal-oxide nanoparticles, such as iron oxides, are used for magnetic resonance imaging[7] and magnetic fluid hyperthermia[8]. Metals, nanosilver and silver nanoalloys in particular, are powerful antibacterial agents[9]. Metal nanoparticles can be surface-modified to increase their biocompatibility and availability[10], they can be conjugated to fluorescent probes to allow for imaging by microscopy techniques, they can be conjugated to drugs and genetic material and functionalized to deliver their cargo to specific target cells[10].

Parallel to the biomedical exploitation of their unique properties, experimental investigations also focus on the assessment of the toxicity of metal NPs[11]. The number of reports on the *in vivo* biodistribution and *in vitro* toxicity of metal nanoparticles keeps increasing. Larger (>10 nm) nanoparticles can accumulate, e.g. in the liver, and determine inflammation and oxidative stress, but the small (<10 nm) nanoparticles are the most cytotoxic[12]. The effect of size is often entangled with the effect of surface functionalization[13,14].