Unravelling mechanism for detecting chromium on functionalized gold nanoparticles *via* a smartphone and spectrophotometric-based systems supported by CIEL*a*b* colour space and molecular dynamics

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The chromaticity diagram

A colour model is a method that humans can create, and specify to visualize colour. RGB colour model is based on the tri-stimulus theory of the human eyes' vision. The RGB colour model describes colours as positive combinations of three appropriately defined red, green, and blue primaries in a Cartesian coordinate system and is an example of an additive colour model.

CIE L*a*b* (or CIELAB) is another colour model that separates the colour information in a way that corresponds to the human visual system. In the CIE L*a*b* colour system L* is defined as lightness; a* and b* are defined as the colour axes to describe the hue and saturation. The colour axes are based on the fact that colour can't be red and green, or both blue and yellow, because these colours oppose each other. The* axis runs from +a which is red to –a which is green and the b* axis from +b which is yellow to –b which is blue. Colour difference in CIE L*a*b* is based on the Euclidean distance between two colours represented in the CIE 1976 CIE L*a*b* uniform colour space. The definition is given by:

$$\Delta E = \sqrt{(\Delta L)^2 + (\Delta a)^2 + (\Delta b)^2} \qquad 1$$

where, ΔL is the difference in lightness/darkness value

Δa is the difference on the red/green axis

Δb is the difference between the yellow/blue axis

Hue angle is the basic unit of colour and is defined as the attribute by which we distinguish red from green, blue from yellow, etc. Chromaticity or chroma is the saturation level or intensity of a particular hue and is defined as the distance of departure of a chromatic colour from the neutral (gray) colour with the same value. Chroma is the vividness or dullness of a colour. Chromaticity increases as a colour become more intense and decrease as colour becomes dull. Both hue and chroma are derived from a* and b* using the following equations:

hue angle: $h = tan^{-1}(\frac{b^*}{a^*})$ 2

chroma: $C^* = \sqrt{(a)^2 + (b)^2}$ 3

1.1 Synthesis of gold nanoparticles

Trisodium citrate capped AuNPs, gold chloride trihydrate solution was prepared by dissolving 0.02 g of the salt in 100 mL deionized water to give a concentration of 0.01 mM. This solution was placed on a hot plate and vigorously stirred using a Teflon-coated magnetic bar. The solution was allowed to boil under constant stirring until it reached the temperature of 96-98 ºC. Thereafter, 5 mL of 0.04 mM warm tri-sodium citrate solution was rapidly added to the boiling solution. A noticeable colour change from pale yellow to wine red was observed within 20 minutes which indicated the formation of AuNPs. The reaction flask was then removed from the hot plate to allow the reaction solution to cool at room temperature.

1.1.1 Fabrication of gold nanoparticles with DPC complex

A 2.0 mM 1.5-diphenylcarbazide (DPC) solution was firstly prepared in ethanol. An aliquot of DPC solution (2 mM, 500 µL) was added with stirring to a solution of citrate-capped AuNPs (0.01 mM, 50 mL).

1.2 Preparation of Cr(VI) standard solutions and their treatment with gold nanoparticles

For the UV-Vis spectrophotometric analysis and image processing, a stock solution of 1000 µM of Cr(VI) was prepared from 1000 ppm stock solution and made to mark in 50 mL with deionized water. The working standard solutions were prepared by dilution of the stock solution with deionized water to get a concentration range of 0.5 to 50 µM. In a 600 µL AuNPs solution, 100 µL HEPES buffer (50 mM, pH 7) and 300 µL of each Cr(VI) standard solution were added.

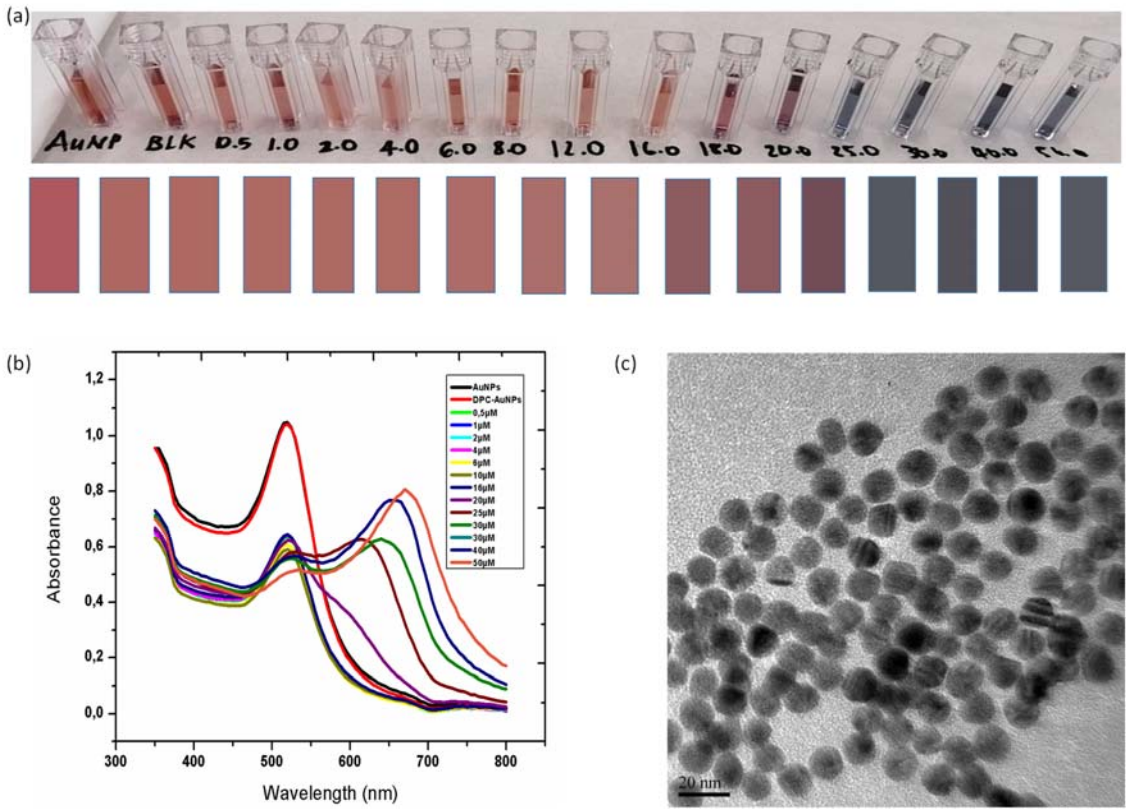


Figure S1: (a) photograph image of the DPC-AuNPs blank and different concentrations of Cr(VI) in the range of 0.5-50.0 µM, (b) concentration-dependent extinction spectra of the DPC-AuNPs blank and different concentrations of Cr(VI) in the range of 0.5-50.0 µM and (c) TEM image of AuNPs sample at 20 nm scale

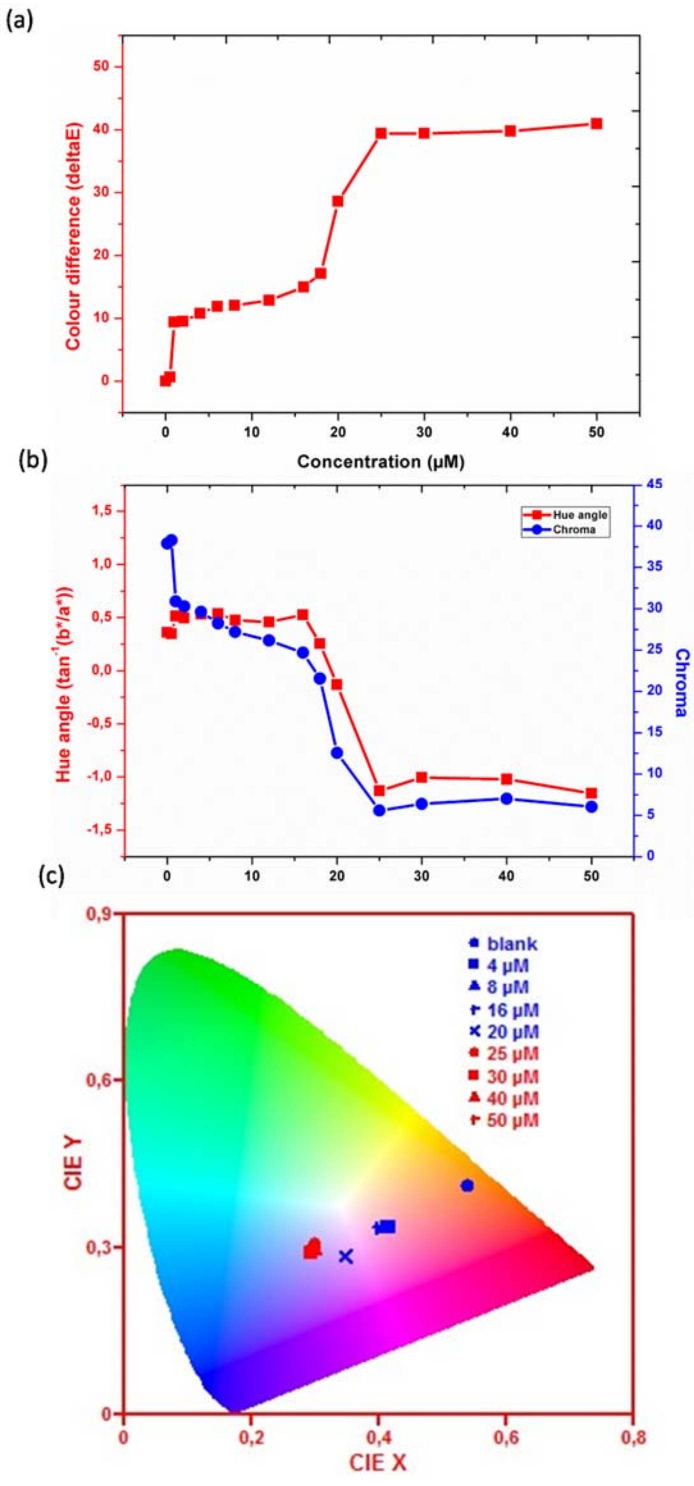
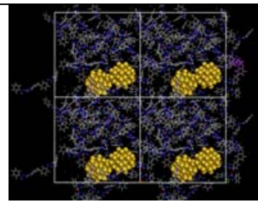
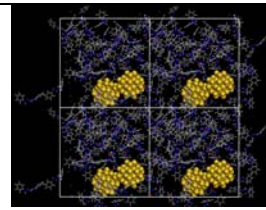
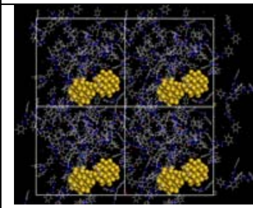
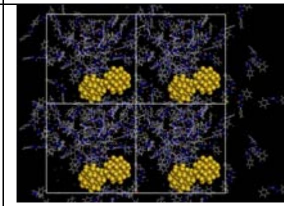
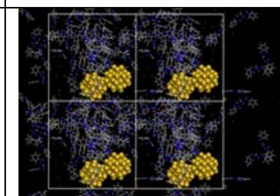
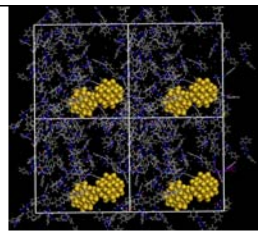
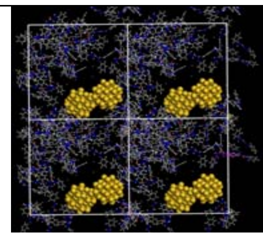
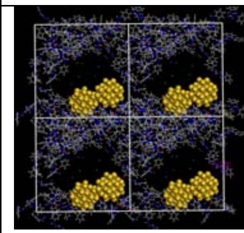
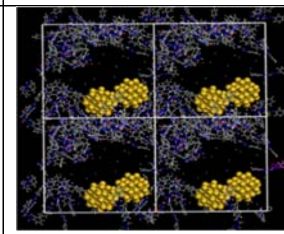
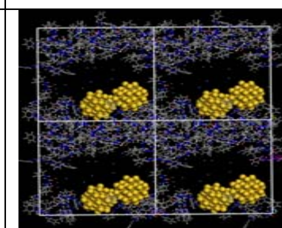
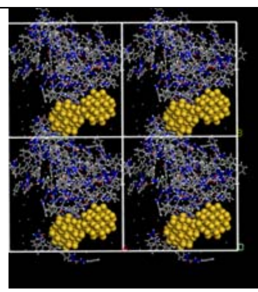
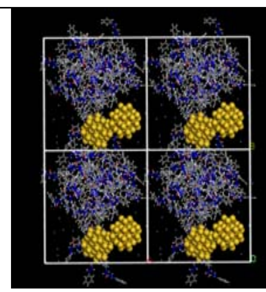
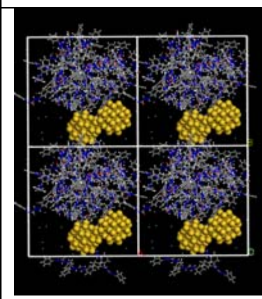
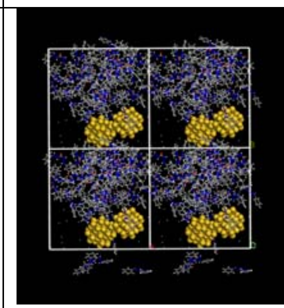
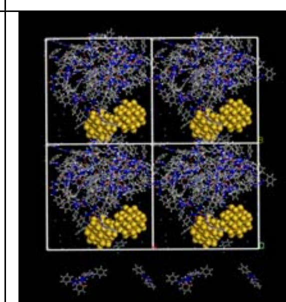


Figure S2: (a) Plot of colour difference against Cr(VI) concentration and (b) Plots of hue angle and chroma values against Cr(VI) concentration, and (c) chromaticity image of calibration standards of Cr(VI)

Table S1: Snapshots for MD simulation performed in triplicate (100 to 500 frames)

MD simulation	**Simulation snapshots (100 to 500 frames)**				
	100	**200**	**300**	**400**	**500**
MD1					
MD2					
MD3					

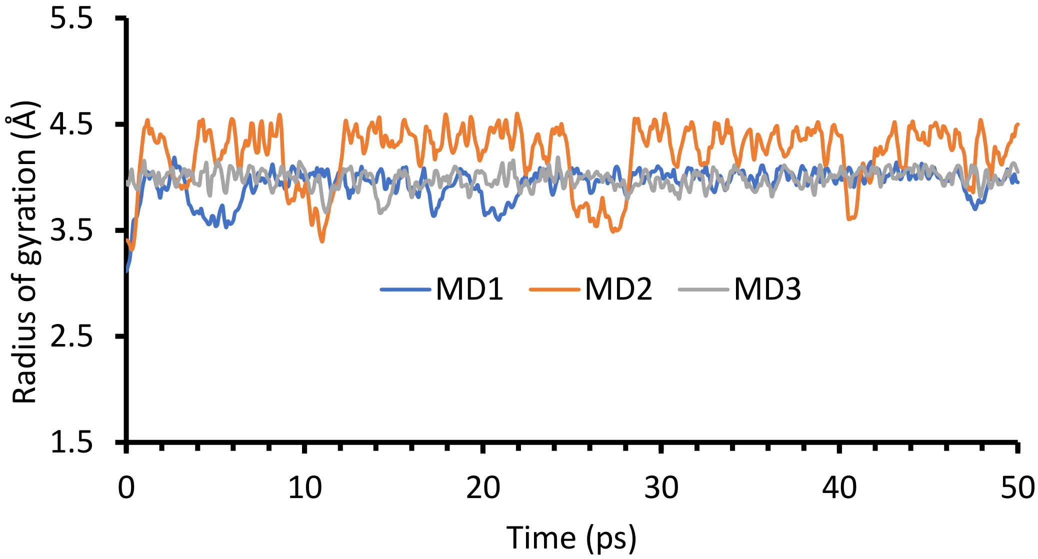


Figure S3: Radius of gyration of MD simulation performed in triplicate