Electronic Supplementary Material (ESI) for Nanoscale Advances.

Supplementary Information

Unveiling the detection kinetics and quantitative analysis of colorimetric sensing for sodium salts using surface-modified Au-nanoparticle probes

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S1 Zeta potentials of AuNPs before and after surface modification

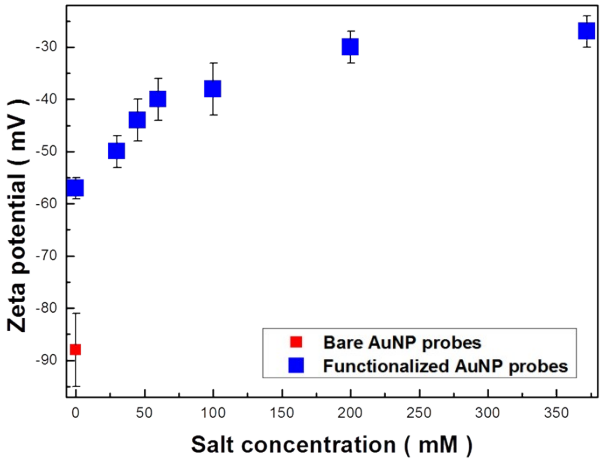

Fig. S1 Measured zeta potentials of bare AuNPs and AuNPs with ascorbic treatment. The variation of zeta potentials of functionalized AuNPs interacted with different salt concentrations were also displayed.

S2 Colorimetric table of detecting Na^+ ions from bare AuNP probes

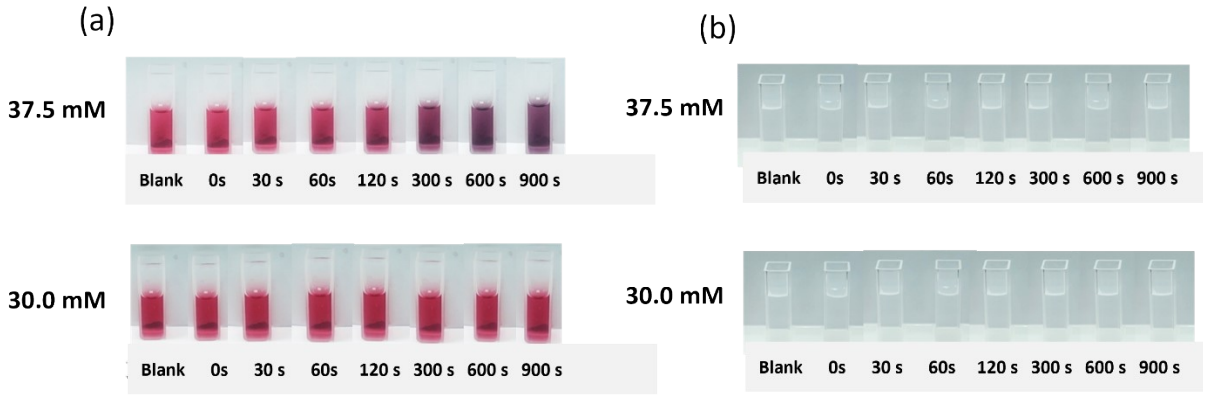

Fig. S2 (a) Colorimetric examinations of detecting Na^+ ions using bare AuNP probes without surface functionalization. The results evidenced the fact that detection sensitivity of bare AuNP probes without conducting ascorbic treatment was comparably low, where they were incapable of detecting 30 mM of Na^+ ions. The colorimetric table in the presence of sodium salts (30 mM and 37.5 mM, respectively) without applying AuNP indicators was presented in Fig. S2(b).

S3 details of FDTD simulation

Numerical investigations of AuNPs were performed using Lumerical software. The proposed AuNPs with radius of 17.4 nm assigned from the results of TEM measurements, were arranged in different aggregation conditions and the simulated AuNP aggregates were surrounded with water. The optical absorbance of AuNPs were examines in the orthogonal cells, where the plane waves were irradiated from Z direction with the wavelength range from 300 nm to 800 nm. The examined system was established by periodic boundary condition in three dimensions, and the unit cell was fixed with dimension of 200 nm on each side. The refractive indices of Au and water are taken from the databases recorded in software.

S4 Selectivity test and applications for practical examinations

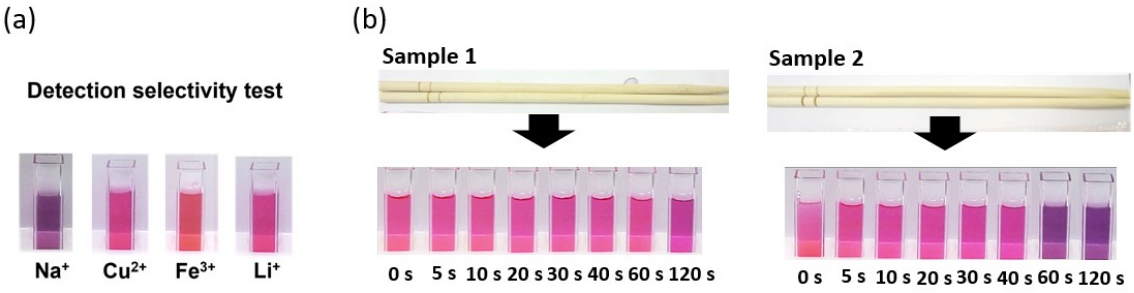

Fig. S3 (a) Photographs of visual sensing in the presence of various metal ions with fixed concentration of 60 mM and detection time of 5 s. (b) Detection of residual Na^+ ions on two different chopsticks using AuNP probes as indicators. The tests were prepared by dipping chopsticks in 100 ml of water for 15 min at 60^0C, and then withdrew 2 ml of tested solutions and mixed them with AuNP probes.

S4 Repetitive utilization of optical sensing

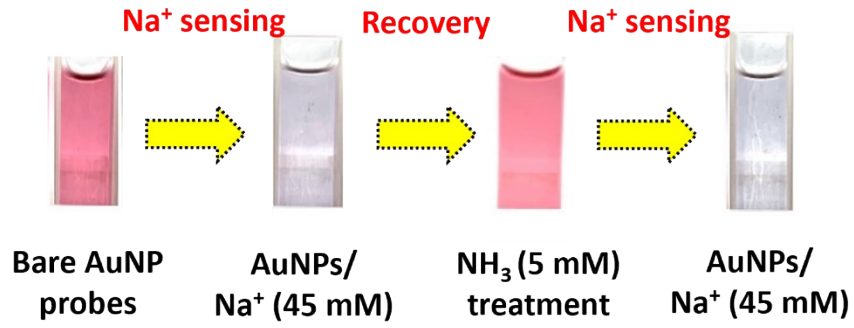

Fig. S4 Colorimetric table of repeated Na+-ion detection using AuNP probes. First, the visual color change could be observed when adding 45 mM of sodium salt in the aqueous AuNP indicators. After that, 1-5 mM of ammonia solutions were introduced to remove the ascorbic acids absorbed on the AuNP surfaces, which would cause the transition of aggregated AuNPs toward dispersed states, and thus the visual color was changed to the original red-wine feature. The repetitive utilization of Na^+-ion detection was again initiated by adding 45 mM of sodium salt in the aqueous AuNP indicators. The obvious color change could be obtained, indicating the sound recovery of AuNP probes through a simple NH_3 treatment.

S5 Explorations of colorimetric detection with RGB color model

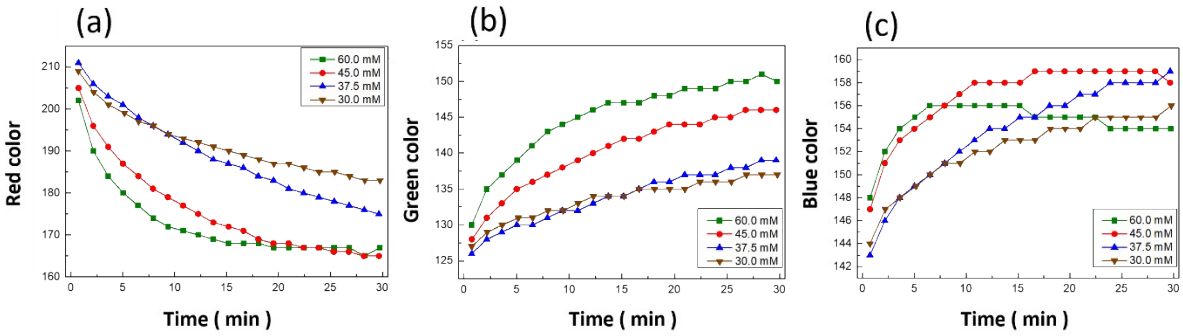

Fig. S5 Examinations of RGB color space considering the variations of present color with respect to salt concentrations (30.0 mM, 37.5 mM, 45.0 mM and 60.0 mM, respectively) and detection time (0-30 min): Deconvolution of color space in (a) red, (b) green and (c) blue. In comparison with the color variations of three examined color spaces, it could be clearly observed that the change in red color space with respect to reaction time (Fig. S4(a)) was the most pronounced case, which represented the dominant component for the realization of visual colorimetric sensing of Na^+ ions.

S6 Stability under light illumination

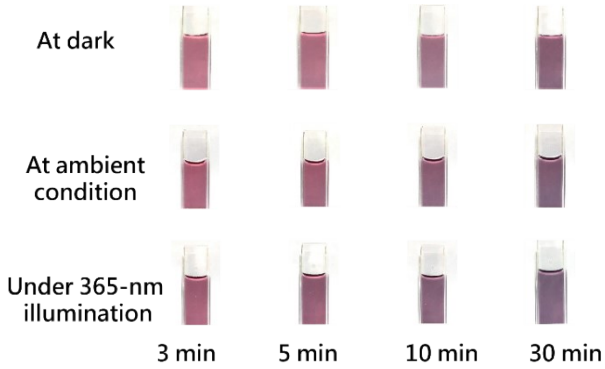

Fig. S6 Exploration of sensing capability at dark, ambient condition and under UV-light illumination (wavelength of 365 nm) for 30 min. The results indicated that the AuNP indicators could be stably utilized for cation detection.

S7 Quantitative analysis by monitoring the light absorbance under the variations of salt concentration and reaction time

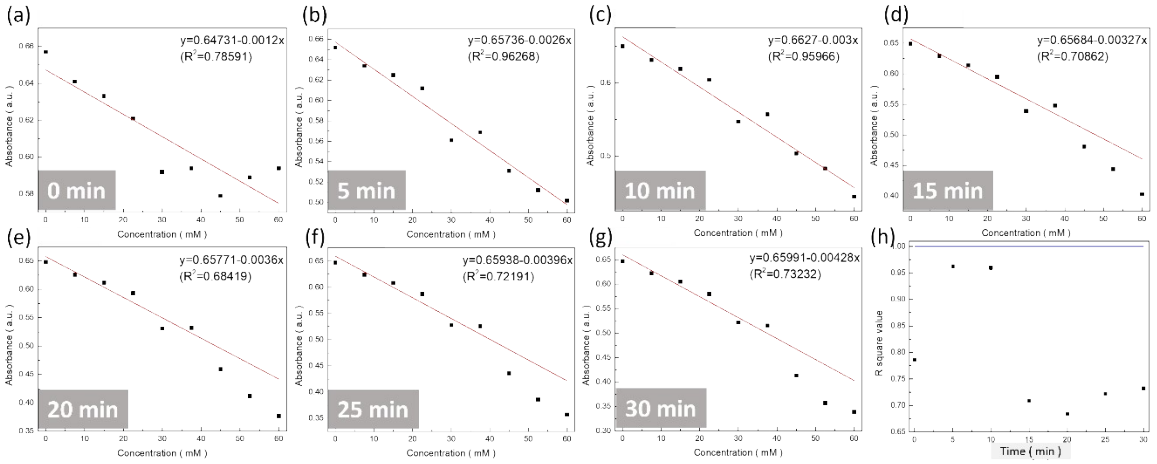

Fig. S7 Experimental expression through the considerations of both light absorbance and reaction time responding to salt concentration by recording absorption intensity at 525 nm with respect to the variations of reaction time: (a) 0 min, (b) 5 min, (c) 10 min, (d) 15 min, (e) 20 min, (f) 25 min and (g) 30 min. (g) The comparative R^2 values under various reaction durations. The findings showed that this model was only workable at short-term detection (< 10 min), while the R^2 values were dramatically reduced to less than 0.75 when detection time was larger than 10 min.

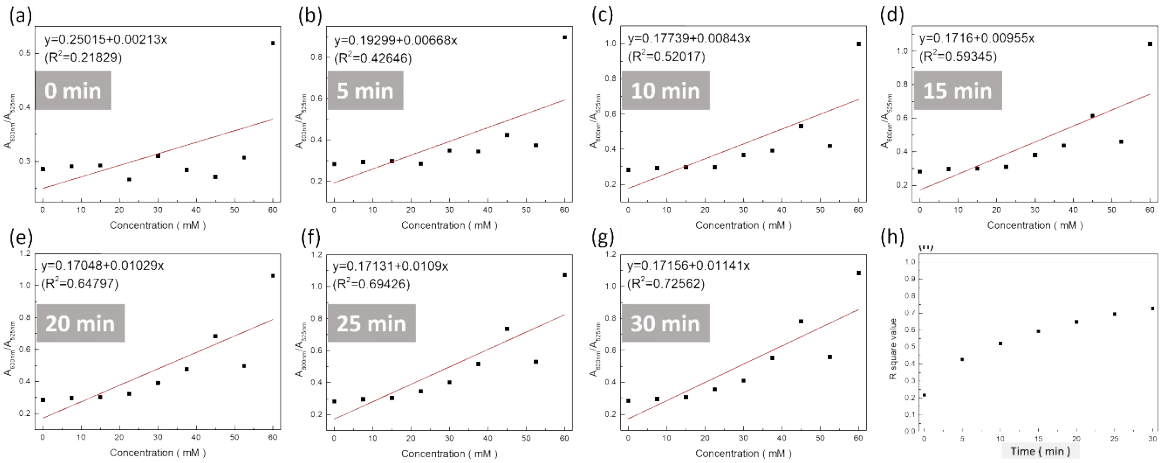

Fig. S8 Experimental expression through the considerations of both light absorbance and reaction time responding to salt concentration by recording intensity ratio of light absorbance at 600 nm to 525 nm with respect to the variations of reaction time: (a) 0 min, (b) 5 min, (c) 10 min, (d) 15 min, (e) 20 min, (f) 25 min and (g) 30 min. (g) The comparative R^2 values under various reaction durations. The results indicated that R^2 values maintained less than 0.8 covering the whole detection durations, which turned to be invalid to express the quantitative analysis of Na^+-ion detection.