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Electronic Supplementary Information (ESI)

Investigation of the *In situ* Generation of Oxide-Free Copper Nanoparticles Using Pulsed-Laser Ablation of Bulk Copper in Aqueous Solutions of the DNA Bases

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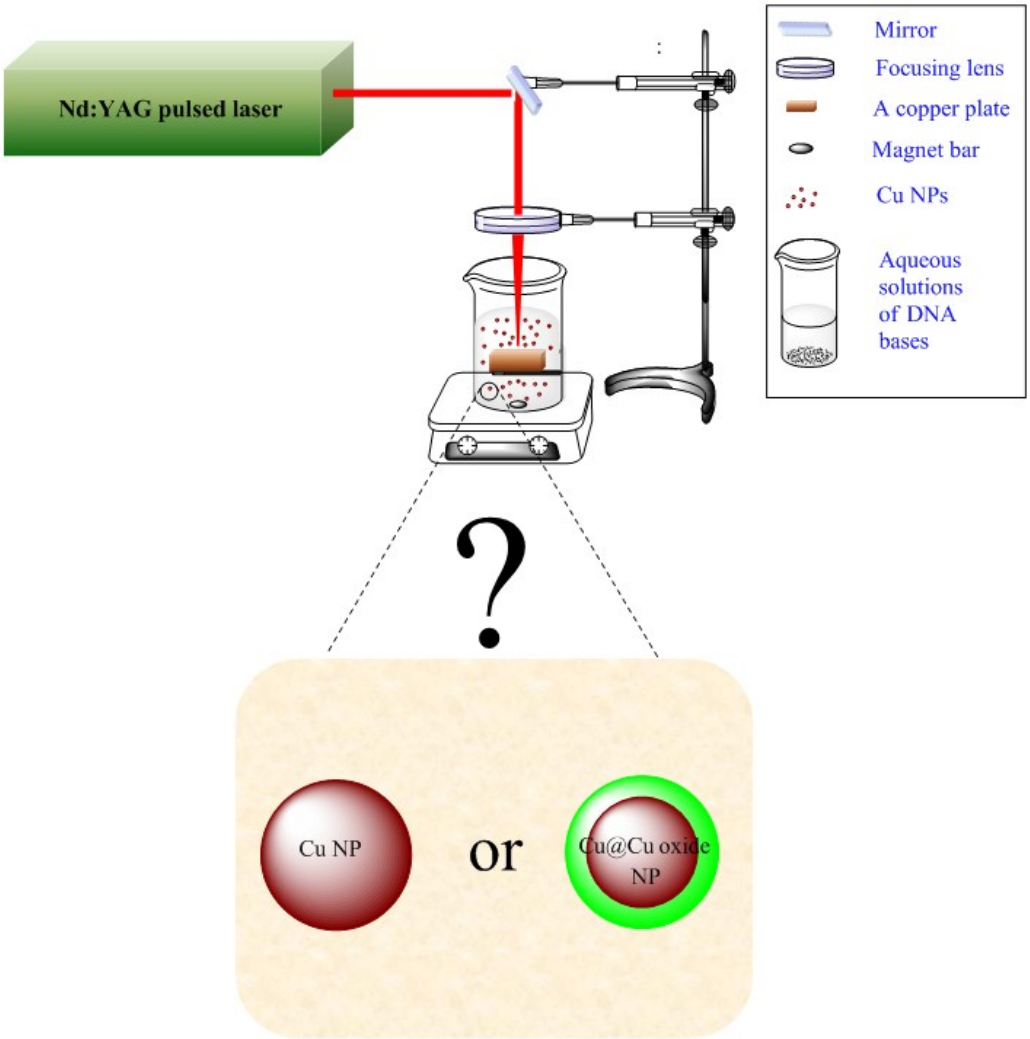

Scheme S1 The general schematic experimental setup used for the preparation of the Cu NPs in aqueous solutions of the DNA bases (adenine, cytosine, and thymine).

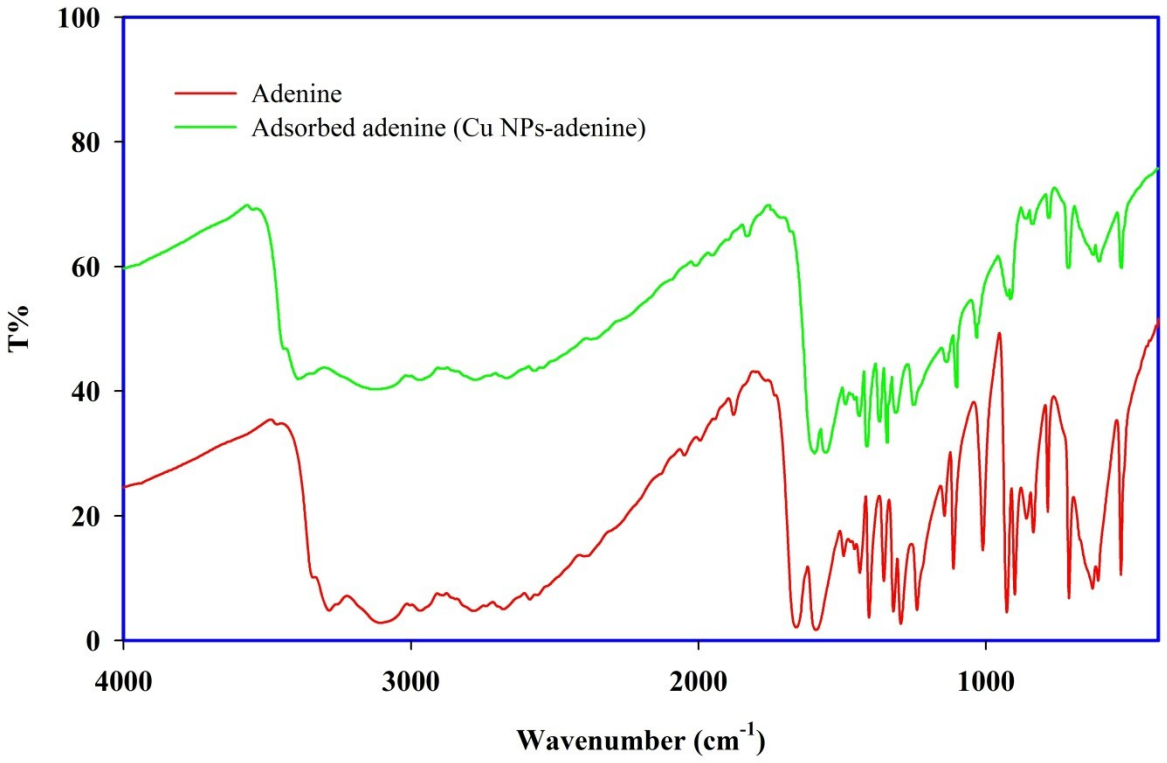

Fig. S1 FT–IR spectra of adenine (red line) and the adsorbed adenine (Cu NPs-adenine) (green line).

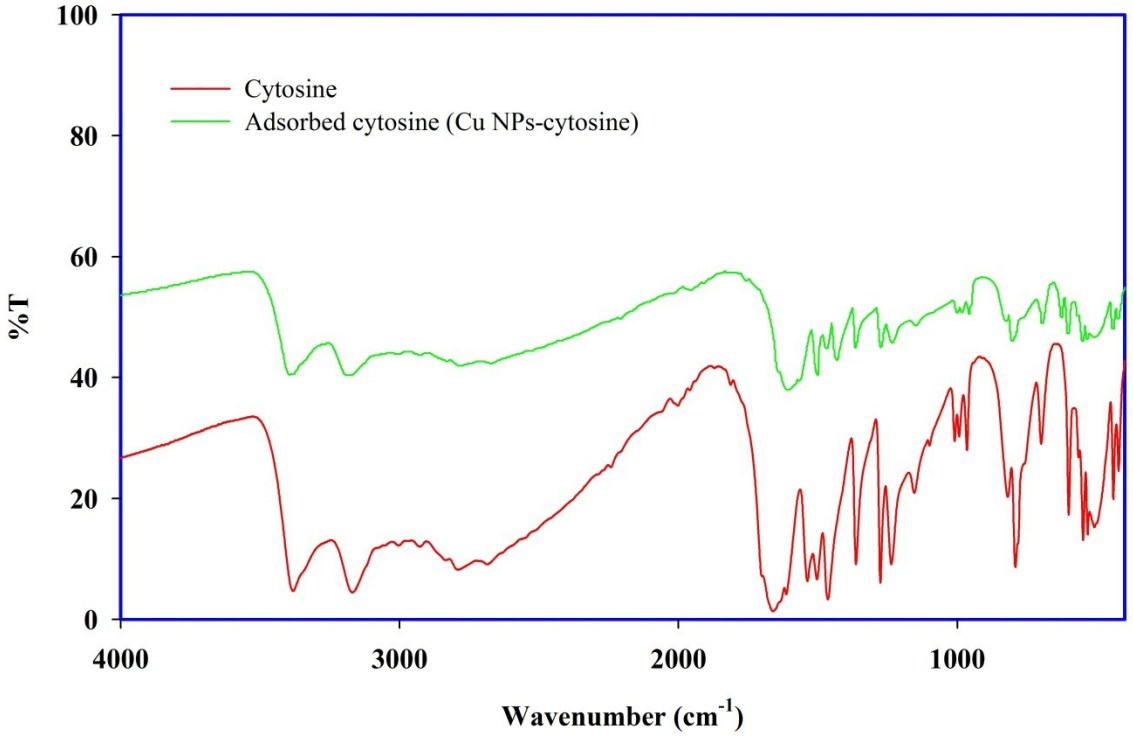

Fig. S2 FT–IR spectra of cytosine (red line) and the adsorbed cytosine (Cu NPs–cytosine) (green line).

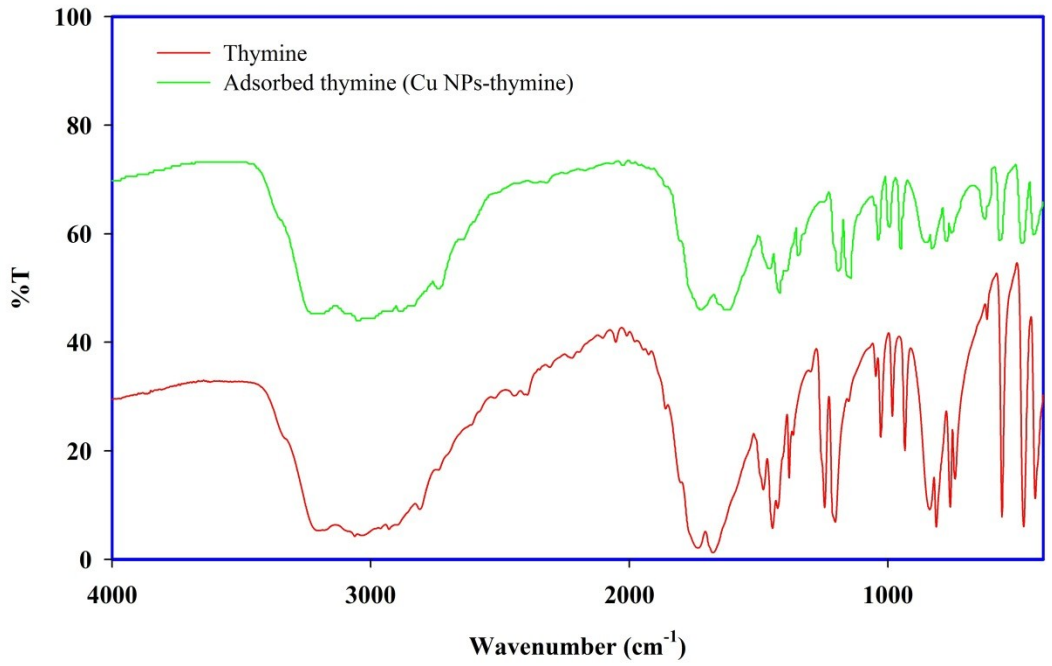

Fig. S3 FT–IR spectra of thymine (red line) and the adsorbed thymine (Cu NPs–thymine) (green line).

Table S1 Main vibrational frequencies of the free and adsorbed adenine.

Modes	Free form (cm^{-1})	Adsorbed form (cm^{-1})
$v(NH_2)$	3287 (asymmetric), 3109 (symmetric)	3396 (asymmetric), 3143 (symmetric)
v(N–H)	1663	1595
v(C–N(7))	1596	1547
v(C–C) v(C–H)	1320	1347
v(C–N) v(C–H)	1238	1252
v(C–C) (in plane) v(C–H) (out of plane)	1111	1099
v(C–C–N)	1012	1027
$v(NH_2)$	925	911

Table S2 Main vibrational frequencies of the free and adsorbed cytosine.

Modes	Free form (cm^{-1})	Adsorbed form (cm^{-1})
$v(NH_2)$	3172	3181
v(C=O)	1657	1617
v(N(3)=C(4))	1543	1495
v(C(5)=C(6))	1460	1439
$v(C(4)–NH_2)$	1365	1376
v(N–C–N)	788	798
Ring breathing of imidazole	698	692

Table S3 Main vibrational frequencies of the free and adsorbed thymine.

Modes	Free form (cm^{-1})	Adsorbed form (cm^{-1})
ν(N(1)–H) ν(N(3)–H)	3050	3061
ν(C(2)=O)	1739	1726
ν(C(4)=O)	1674	1630
δ(NH)	1442	1422
δ(C–O)	1200 1025 932	1148 1040 952
δ(C–H)	736	746

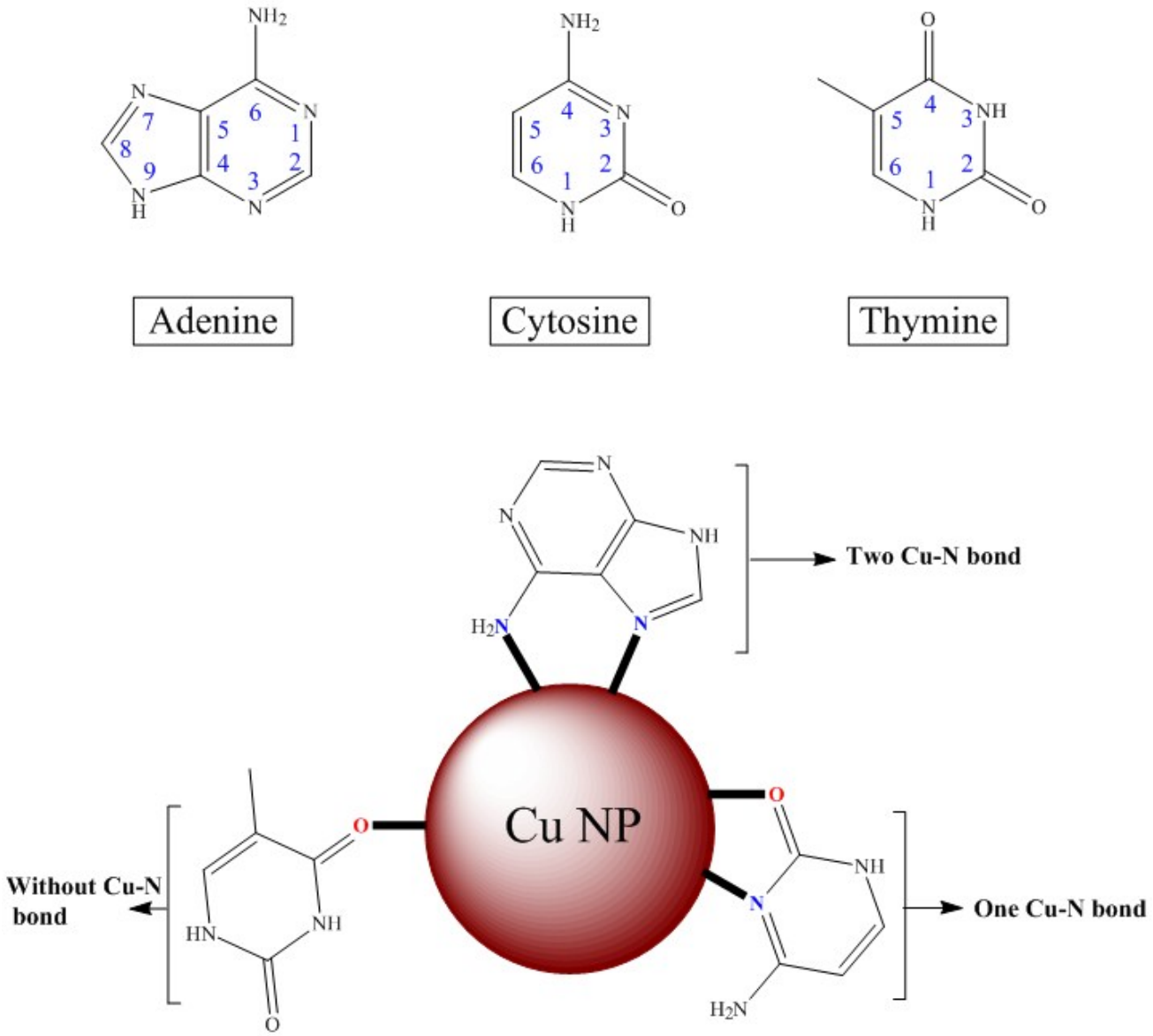

Fig. S4 Structures of three DNA bases (adenine, cytosine, and thymine) and their binding interaction with the copper nanoparticle (Cu NPs). The numbers in the blue color are the positions of the atoms of the bases. The binding interactions are indicated by the black lines.