Supporting Information

Dual Probe Sensors Using Atomically Precise Noble Metal Clusters

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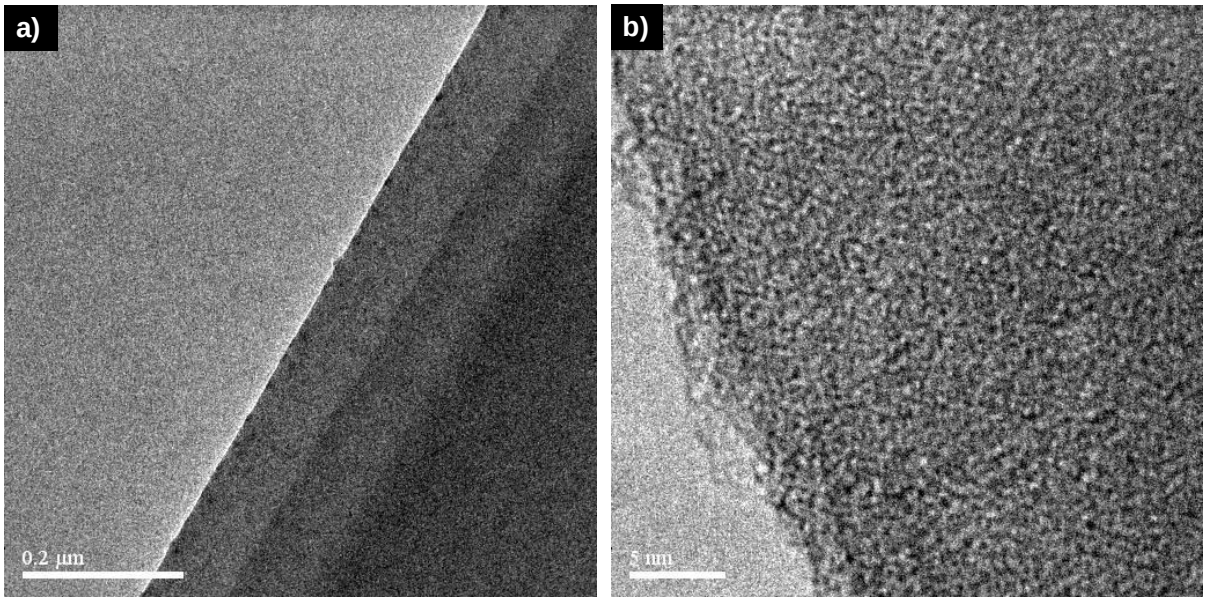

Figure S-1. TEM of the calcined fibers at different magnifications.

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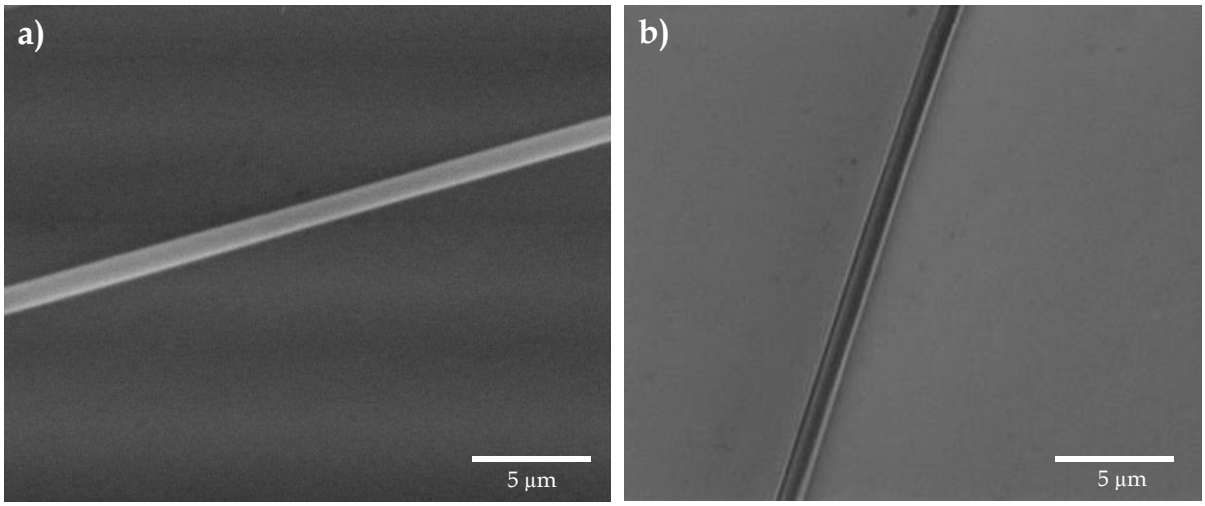

Figure S-2. SEM of the fibers: a) before carbonization and b) after carbonization.

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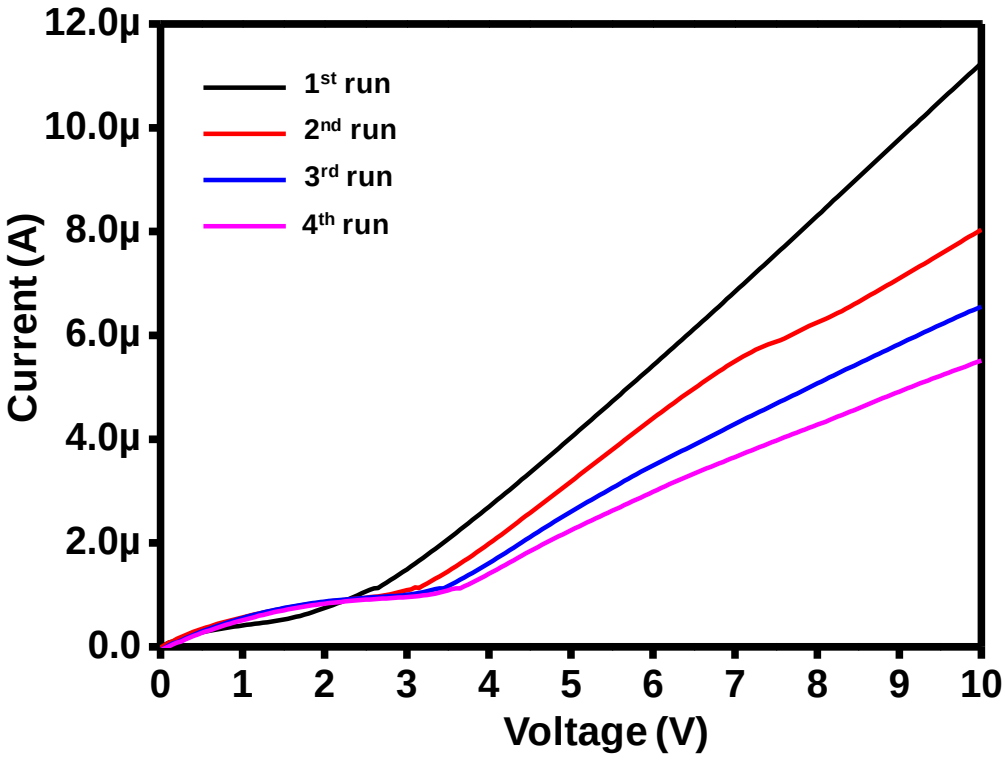

Figure S-3. I-V studies of fiber coated with BSA.

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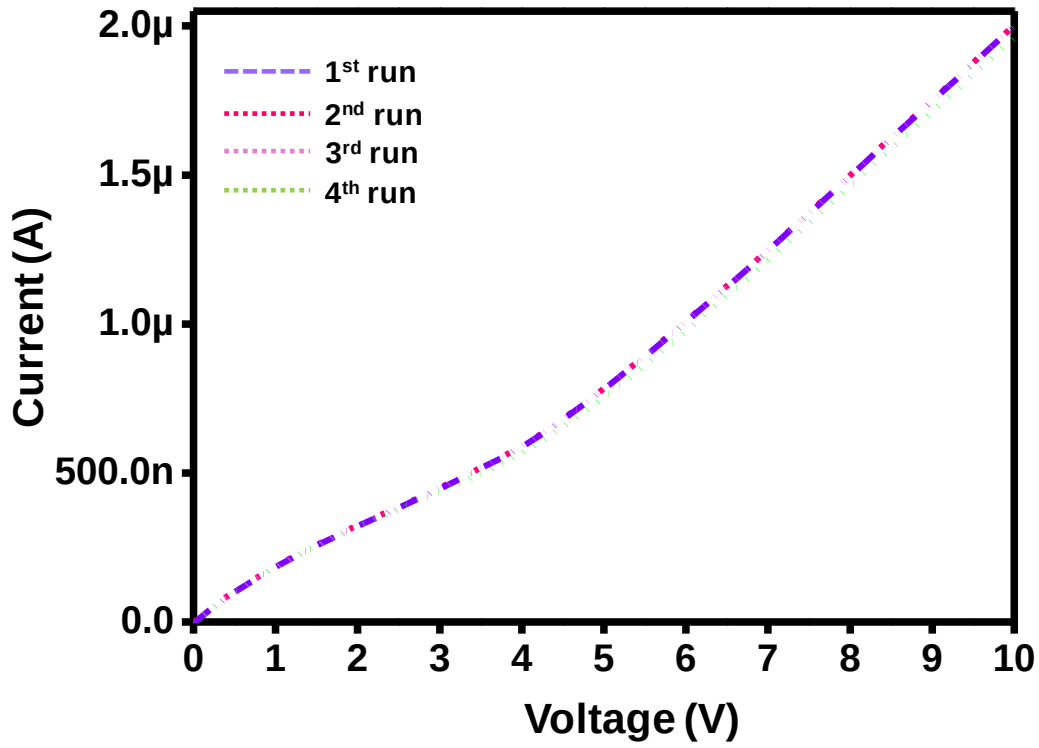

Figure S-4. I-V studies of cluster coated fiber.

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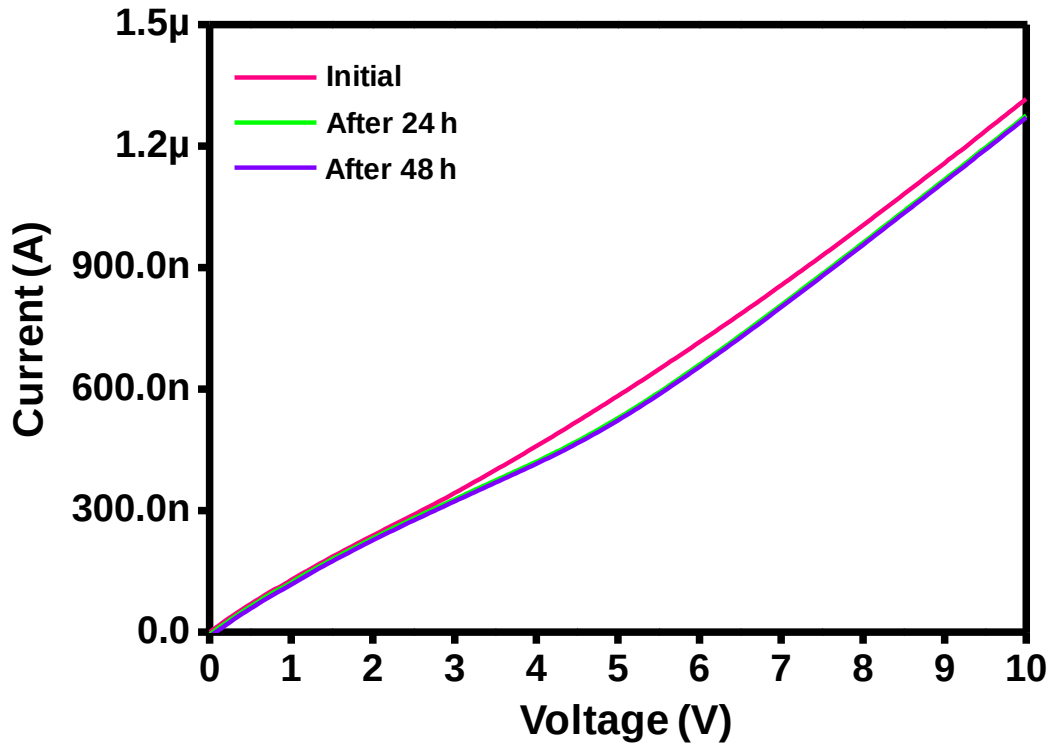

Figure S-5. I-V studies of cluster coated fiber at different time intervals.

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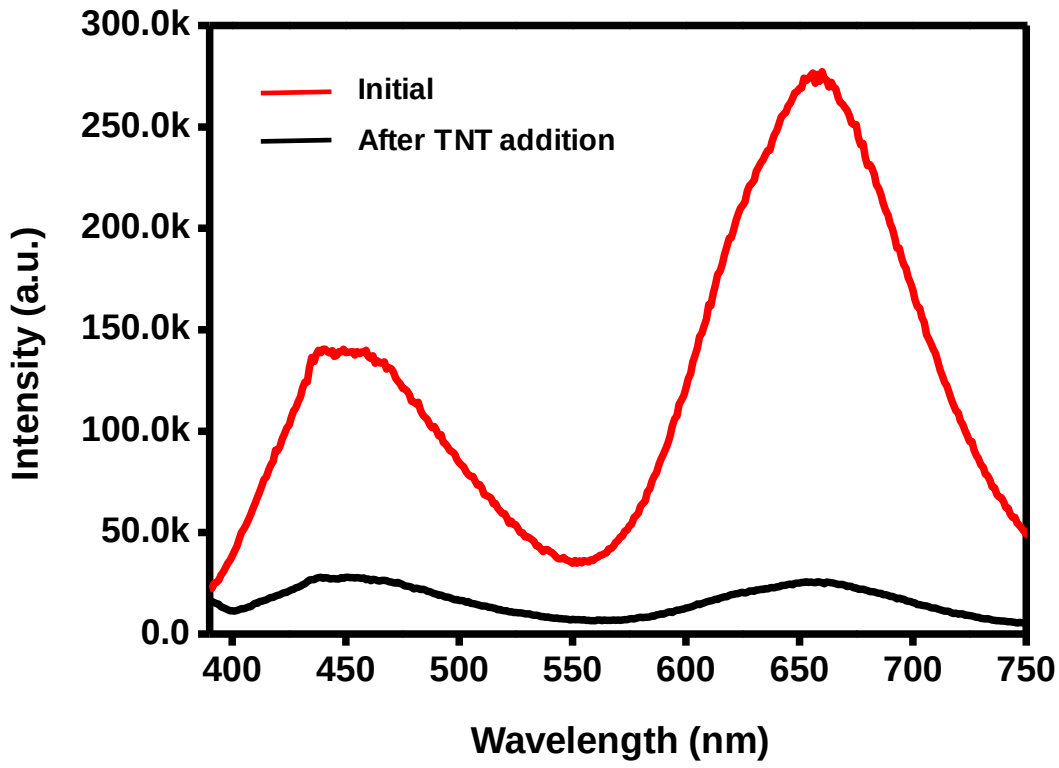

Figure S-6. Photoluminescence profile of Au@BSA cluster after addition of 100 µL of 100 ppt TNT to 2 mL of Au@BSA cluster solution.

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Details of the calculation for solution based fluorescence experiments

For the fluorescence experiments, 2.5 µL of water is drop casted onto the slide containing and the measurements were done. The area of droplet measured is 8.34×10^{-6} m^2.

1 ppt of analyte= 4.403×10^{-12} M TNT

No. of molecules per litre = $4.403 \times 10^{-12} \times 6.023 \times 10^{23}$

$= 2.652 \times 10^{12}$

Hence,

2.5 µL of water droplet contains = $2.5 \times 10^{-6} \times 2.652 \times 10^{12}$

$= 6.625 \times 10^{6}$ TNT molecules

Surface area of a fiber = $2\pi rh$ Fiber radius = 600 nm

Fiber length = 40 µm

$= 2 \times 3.14 \times 6 \times 10^{-7} \times 4 \times 10^{-5}$ m^2

$= 1.5 \times 10^{-10}$ m^2

8.34×10^{-6} m^2 (2.5 µL of water droplet) contains 6.625×10^{6} TNT molecules

Hence,

1.5×10^{-10} m^2 (single fiber) contains = 1.5×10^{-10} $m^2 \times 6.625 \times 10^{6} / 8.34 \times 10^{-6}$

= 119 TNT molecules

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Details of the calculation for TNT vapor exposure experiments

TNT powder was placed in a beaker as shown in Figure 4.
Beaker, height = 3.5×10^{-3} m
Radius = 1.1×10^{-3} m
Volume of the beaker = $\pi r^2 h$
= 13.297×10^{-9} m^3
Surface area of a fiber = $2\pi rh$ Fiber radius = 600 nm
Fiber length = 1 mm
=$2 \times 3.14 \times 600 \times 10^{-9} \times 1 \times 10^{-3}$
= 3.768×10^{-9} m^2

To calculate the number of TNT molecules in the beaker at 343.15 K
Gas equation, PV = nRT
Here,
P is taken as the vapor pressure,
Hence, P = 4.24 Pa (From literature), V = 13.297×10^{-9} m^3
R = 8.314, T = 343.15 K

Therefore,
n = $4.24 \times 13.297 \times 10^{-9} / 8.314 \times 343.15$
= 1.97×10^{-13}
Hence,
Number of molecules present in the beaker = $1.97 \times 10^{-13} \times 6.023 \times 10^{23}$
= 1.19×10^{12}
= ~ 10^{12} TNT molecules
To calculate the number of TNT molecules for monolayer coverage on the fiber
Size of TNT molecule, d = 1 nm
Number of molecules required for mono layer coverage = Surface area / πr^2
= $3.768 \times 10^{-9} / 3.14 \times (0.5 \times 10^{-9})^2$
= 4.8×10^9 molecules of TNT
4.8×10^9 molecules of TNT are required for a uniform monolayer coverage for 1 mm length fiber.

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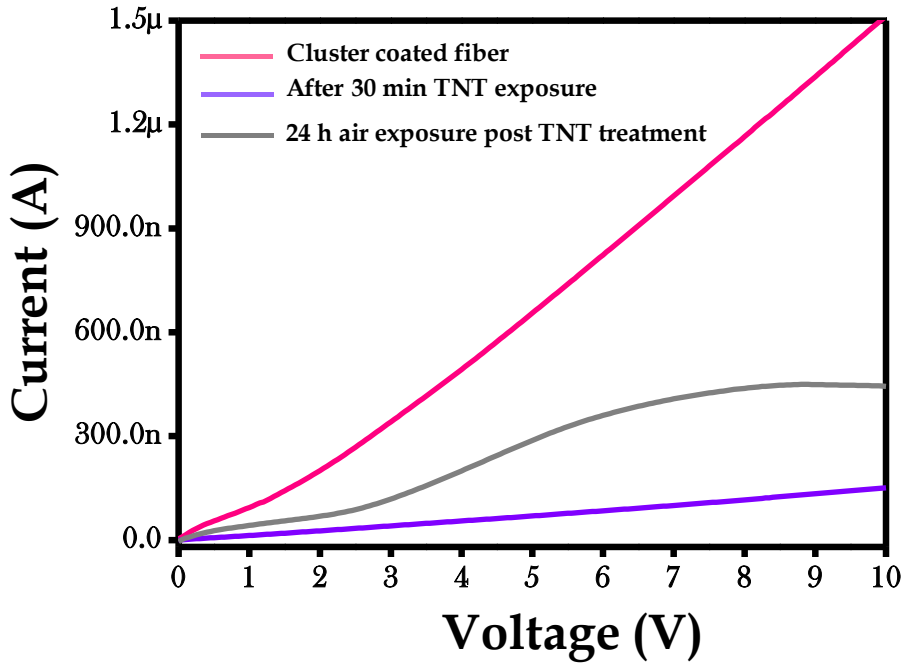

Figure S-9. I-V studies of cluster coated fiber.

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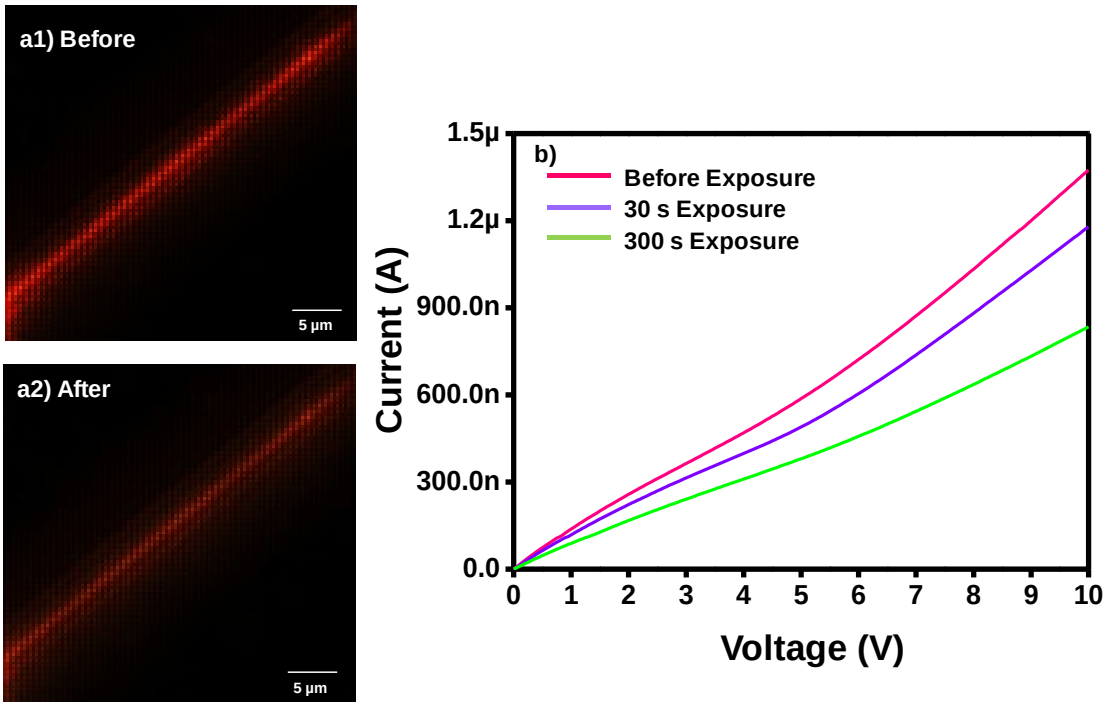

Figure S-10. Flourescence image of the fibers, a1) before exposure to DNT, a2) after exposure to DNT for 30s, b) I-V studies of cluster coated fiber exposed to DNT.

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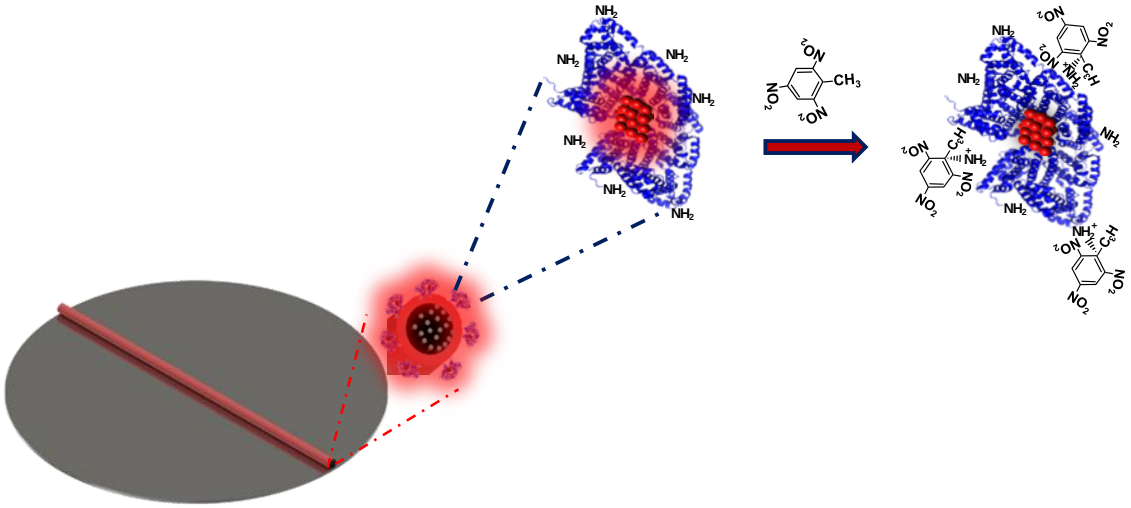

Figure S-11. Schematic representing the formation of Meisenheimer complex between the nitro groups of TNTand the free amino groups of BSA of the Au@BSA cluster immobilised on CNTs@SiO_2 fibers.