

Supplementary Material

Here we explore the *%Diff* at the physical stage between a cluster of GNPs and an heterogeneous MixNP, modelled as a two concentric spheres as shown in Fig. S1, where the gold/water mixture is surrounded by water cell.

The setting of the properties of the inner sphere for the heterogeneous MixNP were set *a posteriori*, by sampling it's density and radius, and choosing the parameters that minimizes the *%Diff* of the Radial Dose Distributions (RDDs) with respect to the GNPs cluster. The best set of parameters are shown in Table S1. Using those values, the DEF and *%Diff* for the all sizes of the heterogeneous MixNP are plotted in Fig. S2.

To show the drastic improvement on the *%Diff* by the hereogenous MixNP, Fig. S3 shows a comparison of the *%Diff* between a full GNPs cluster versus the homogeneous and heterogeneous MixNP.

Table S1. Set of optimized parameters used to model the heterogeneous MixNP for all sizes.

MixNP size (nm)	Density (g/cm3)	Core radius (nm)
70	8.767	64
250	7.895	240
500	7.9	480

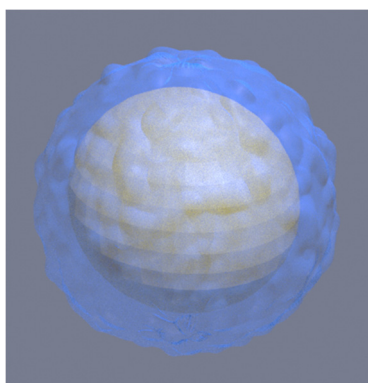


Figure S1. Visualization of the heterogeneous MixNP, showing a water cell surrounding an homogeneous mixture of gold and water.

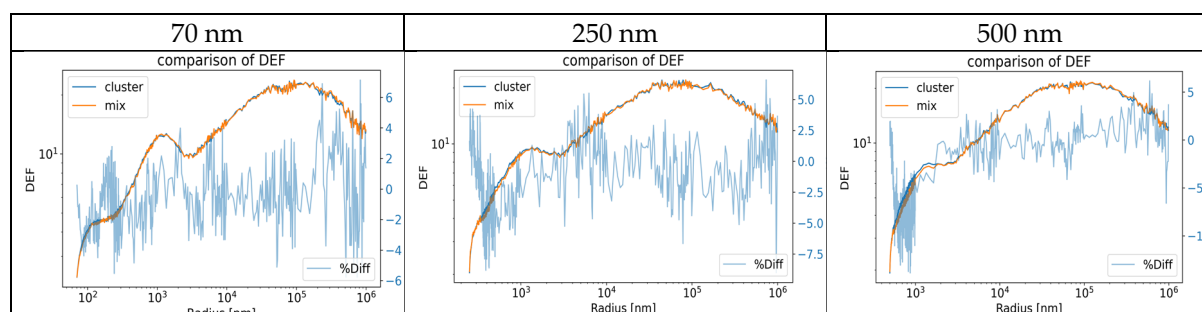


Figure S2. DEF and *%Diff* (blue) between the cluster and the heterogeneous MixNP for all sizes.

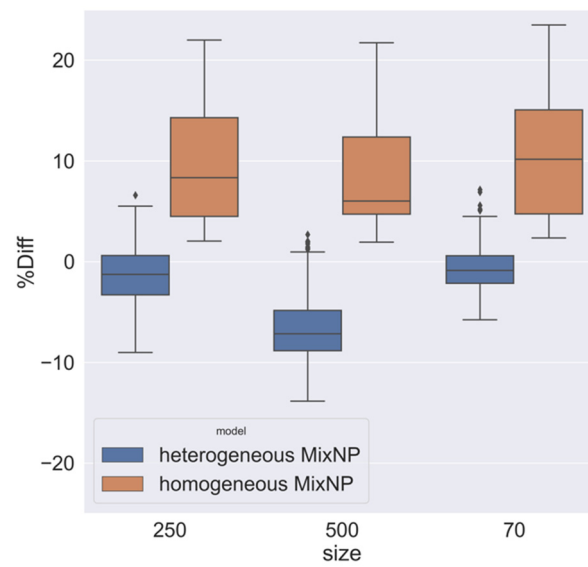


Figure S3. Boxplot comparing the %Diff between the cluster and the heterogenous/homogeneous MixNP for all sizes.