Supporting Information

Strong dependence of surface plasmon resonance and surface enhanced Raman scattering on the composition of Au-Fe nanoalloys

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Figure S1. Numerical calculations (with the DDA method) of the extinction cross section (σ_{ext}) for Au nanospheres (26nm in diameter) in water embedding 6 grains of metal iron or iron oxide of variable size, each occupying the six vertex of an octahedron. Two different cases are considered: grains tangent to the surface of the Au nanosphere (a) or grains at 3nm from the surface of the Au nanosphere (b). The size of the grains is varied in order to give a progressively increasing iron fraction (x) in the Au nanosphere, as reported in the plots’ labels. Figures (c) and (d) refer to metal iron grains, figures (d) and (f) to iron oxide grains (iron(II,III) oxide or magnetite). The σ_{ext} are normalized to the value at 400nm for the sake of comparison with experimental spectra. There is no correspondence between calculated and experimental optical spectra, thus excluding that Au-Fe nanoparticles are constituted by segregated phases.
Figure S2. We tested the effect of Ar\(^+\) sputtering on surface oxidised Fe species of an iron oxide commercial powder (Iron(II,III) oxide powder, Sigma-Aldrich product no.310069). The BE of the Fe 2p peak does not change after 10’ of sputtering, whereas a shift of only 0.5 eV is observed after 20’ of treatment. In all cases, the BE of the oxidised Fe species does not match that measured for the same Fe 2p peak in Au-Fe nanoalloys sputtered for 10’.