**Laser/Plasma Assisted Synthesis of Gold-Iron Nanoparticles and Laser Desorption Ionisation for Generation of Au*m*Fe*n+/-* (*m* = 1-35; *n* = 1-3) Clusters**

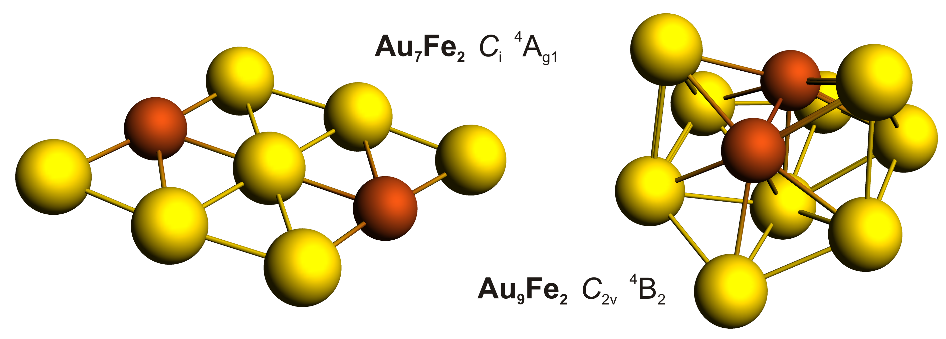
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Gold-iron or gold-iron oxide nano-particles (NPs) are of particular importance because of their bio diagnostic and medicinal applications. Applying either plasma (8.3 kHz) or electrochemically we produced a kind of Au-Fe nano-composite, in case of plasma a giant gold nano-flowers (1-2 000 nm). The product was analysed by EDX and SEM. Mass spectrometry with LDI (laser 337 nm) yields single charged Au*m*Fe*n*± (*m* = 1-35; *n* = 1-3) clusters. Structures of clusters in neutral and mono-charged forms were designed by DFT calculations (ADF; scalar relativistic ZORA geometry optimization). The structures in local minima of potential energy surface always have Fe atoms coordinated to several Au atoms (most often to 4 to 6) and possess few odd electrons (4 to 9). The distances of a Fe nucleus from adjacent Au nuclei lie in the interval 2.5 – 2.7 Å.



References:

1] Ravi Madhukar Mawale, Mayuri Vilas Ausekar, David Pavliňák, Oleksandr Galmiz, Pavel Kubáček, Josef Havel, Laser Desorption Ionization Quadrupole Ion Trap Time-of-Flight Mass Spectrometry of Au*m*Fe*n*+/- Clusters Generated from Gold-Iron Nanoparticles and their Giant Nanoflowers. Electrochemical and/or Plasma Assisted Synthesis. J. Am. Soc. Mass Spectrom. (2016).

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