

# Electron production by noble metal nanoparticles in collision processes with photons and fast ions

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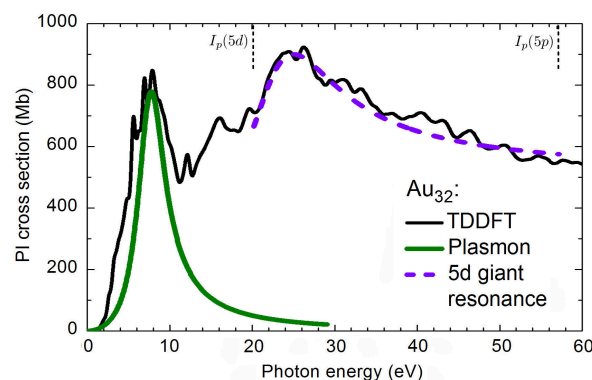
**Synopsis** We analyzed electron production by noble metal nanoparticles irradiated by photons and fast ions. For that, photoabsorption spectra of several gold clusters were calculated in a broad photon energy range by means of time-dependent density-functional theory (TDDFT). Two dominant peaks appearing in the spectra of electron emission of noble metal clusters were assigned to two distinct types of collective electron excitations. This study revealed that the decay of the collective excitations formed in the nanoparticles is an important mechanism of generation of low-energy electrons, which are known to act as important agents of biodamage.

It is currently acknowledged that low-energy secondary electrons (having the kinetic energy from a few eV to several tens of eV) and other species, which are produced when fast ions propagate through a biological medium, largely cause the biological damage [1, 2]. As was proposed recently, cancer treatments with ionizing radiation can be improved by injecting metal (noble metal, in particular) nanoparticles which may increase the number of secondary species in the target region. However, the nanoscale mechanisms leading to an improvement of existing techniques are still to be thoroughly substantiated.

We performed a theoretical and numerical analysis of electron production by noble metal (gold, platinum, silver) nanoparticles irradiated by photons and fast ions. For that, we calculated the photoabsorption spectra of  $Au_N$  ( $N = 18 - 42$ ) clusters in a broad photon energy range by means of the TDDFT approach. Two prominent features of the spectra were assigned to the two distinct types of collective electron excitations (Fig. 1). Plasmons, i.e. collective excitations of delocalized valence electrons, dominate the spectra of electron emission from metallic nanoparticles in the energy range of about 1 – 10 eV. For higher electron energies (of a few tens of eV), the main contribution to the electron yield arises from the atomic giant resonance associated with the collective excitation of 5d electrons in individual atoms of a nanoparticle.

Similar to the photoionization, the two distinct types of collective electron excitations appear in the process of impact ionization. We demonstrated that noble metal nanoparticles, especially those made of gold and platinum, significantly enhance the electron yield due to the collective response to an external electric field of a charged projectile. As a result of these effects,

the number of the low-energy electrons generated by small noble metal nanoparticles significantly exceeds that produced by an equivalent volume of water [3, 4]. Thus, decay of the collective electron excitations formed in the nanoparticles represents an important mechanism of generation of the low-energy electrons.



**Figure 1.** Photoabsorption cross section of the  $Au_{32}$  cluster calculated within TDDFT (thin curve). Thick solid and dashed curves represent the contributions of the plasmon-type and the localized (giant resonance) excitations, respectively [3, 4]. Vertical lines mark the 5d and 5p ionization thresholds in the atom of gold.

## References

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