# Noble Metal Nanoclusters: Tiny Structures, Big Impact

**Martina Perić Bakulić**

*martina.peric-bakulic@ktf-split.hr*

*Faculty of Chemistry and Technology, University of Split, Ruđera Boškovića 35, 21000, Split, Croatia*

Nanoscience, followed closely by computational chemistry, has emerged as a powerful and valuable research avenue in recent decades [1, 2]. This is largely due to the unique physical phenomena observed at the nanoscale between 1 and 100 nm, which aligns with Richard Feynman's visionary idea of manipulating matter at the atomic level, as famously presented in his lecture *"There's Plenty of Room at the Bottom"* [3].

Within this scale, atomically precise noble metal nanoclusters (NCs) have gained significant attention, particularly for biomedical applications. Gold and silver NCs, in particular, stand out due to their ultra-small size, excellent biocompatibility, intense photoluminescence, low toxicity, and photostability. However, their standalone use in bioimaging is limited, as they tend to degrade in biological environments, losing both structural integrity and optical function.

To overcome this, functionalization with biomolecules plays a critical role. Such surface modifications not only stabilize the NCs but also enhance their emission properties, reduce toxicity, and enable specific target recognition - essential for effective biosensing. This presentation focuses on the optical properties of noble metal NCs , aiming to explore their dual potential: enhancing light-harvesting capabilities for solar energy applications, and enabling advanced bioimaging properties. Special emphasis is placed on integrating noble metal NCs with organic dyes and tailored ligands.

Time-dependent density functional theory (TDDFT) serves as a key theoretical approach, providing insight into the origins of optical properties in both liganded NCs and bio-nano hybrids of noble metals, guiding the design of multifunctional nanomaterials [4-7].

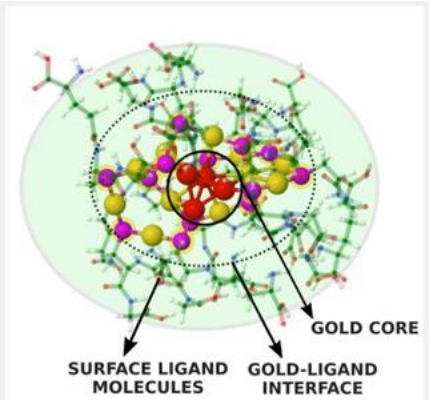


**Figure 1.** Schematic representation of gold nanocluster as a multishell system [5]

## References:

[1] Nanoscience and Nanotechnologies: Opportunities and Uncertainties, Royal Society policy document. Royal Society, 2004.

[2] M. Vestergaard, K. Kerman, I. Hsing, E. Tamiya, Nanobiosensors and Nanobioanalyses, Springer Japan, 2015.

[3] R. P. Feynman, *Caltech Engineering and Science* **23** (1960) 22-36.

[4] M. Perić, Ž. Sanader Maršić, I. Russier-Antoine, H. Fakhouri, F. Bertorelle, P.-F. Brevet, X. le Guével, R. Antoine, V. Bonačić-Koutecký, *Phys. Chem. Chem. Phys*. **21** (2019) 23916-23921.

[5] M. Perić Bakulić, Design of new nanostructured materials for application in biosensorics; theoretical study of optical properties of noble metal bio-nano hybrids, PhD thesis, University of Split, Faculty of Science, 2022.

[6] M. Bužančić Milosavljević, A. Mravak, M. Perić Bakulić, V. Bonačić-Koutecký, *RSC Adv*. **13** (2023) 6010-6016.

[7] H. Yuan, I. Russier-Antoine, C. Moulin, P.-F. Brevet, Ž. Sanader Maršić, M. Perić Bakulić, X. Kang, R. Antoine, M. Zhu, *Nanoscale Horiz*. **10** (2025) 314-321.