Engineering Alloy Nanoclusters in a Cellulose Matrix for Enhanced Type-I Photodynamic Theranostics

*Negar Hosseiniyan [a], Pietro Castronovo [b], Gregory Beaune [a], Eslam Abdelrady [c], Xi Chen [a], Artem Zhyvolozhnyi [c], Hamza Siddiqui [c], Hua Jiang [a], Minna Makki [a], Marco Cannas [b], Alice Sciortino [b], Ilya Skovorodkin [c], Anatoliy Samoylenko [c], Seppo J. Vainio [c], Fabrizio Messina [b] *, and Sourov Chandra [a] **

[a] *Department of Applied Physics, Aalto University, FI-00076 Espoo, Finland,* [b]*Dipartimento di Fisica e Chimica Emilio Segre`, Universita`degli Studi di Palermo, 90123 Palermo, Italy; ATeN Center, Universita`degli studi di Palermo, 90128 Palermo, Italy,* [c] *Laboratory of Developmental Biology, Disease Networks Research Unit, Faculty of Biochemistry and Molecular Medicine, Infotech Oulu, Kvantum Institute, Oulu University, 90014 Oulu, Finland*

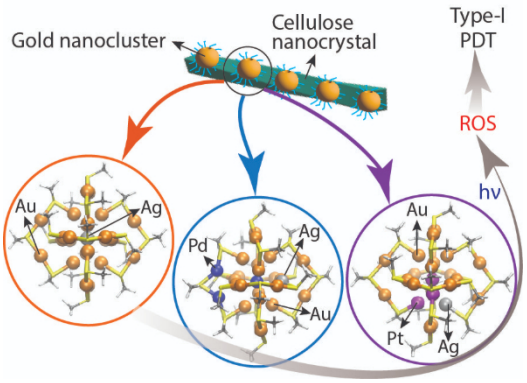
negar.hosseiniyan@aalto.fi

Photodynamic therapy (PDT) has emerged as a minimally invasive strategy for cancer treatment. However, its clinical translation is limited by oxygen dependence, poor selectivity, and suboptimal photosensitizer performance. [1] In particular, conventional organic photosensitizers suffer from low solubility, limited tissue penetration, and phototoxic side effects, while many inorganic alternatives raise concerns regarding long-term toxicity and biocompatibility. [1]

Atomically precise gold nanoclusters (AuNCs) have emerged as an active area of great interest due to their ultra-small size (usually < 2 nm), discrete energy levels and most importantly their intrinsic biocompatibility. [2] They are behaving in between the atoms and metal nanoparticles. Unlike plasmonic gold nanoparticles, structural control of the Au-cores in AuNCs generates specific bandgaps. As a result, AuNCs exhibit tunable optical properties that make them promising candidates for light-driven biomedical applications, particularly in the realm of imaging, sensing and theranostics. [3]

Herin, we report a versatile theranostic platform based on bioderived cellulose nanocrystal–supported AuNCs (CNC–AuNCs) with selective mono- and multi-heteroatom (Ag, Pd, and Pt) substitution as Type-I photosensitizers. Heteroatom incorporation modulates photoluminescence and excited-state relaxation kinetics while maintaining high biocompatibility. Under light irradiation, nanocluster excited-state pathways enable efficient reactive oxygen species (ROS) generation, leading to effective Type-I photodynamic cell destruction. This approach doesn't rely on external oxygenation and may potentially be effective on hypoxia-responsive imaging and photodynamic therapy.

Keywords:
Gold nanoclusters, Cellulose nanocrystals, Photosensitizer, ROS, Theranostics



Trace heteroatom doping in CNC-supported gold nanoclusters enable efficient Type-I photodynamic theranostics.

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