

# UNIVERSITY OF CALIFORNIA, IRVINE

## DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING

**SPECIAL SEMINAR**

*HOST: STACY COPP*

### ***ATOMIC-LEVEL TUNING OF GOLD NANOCLUSTERS FOR TARGETED CANCER THERAPY***



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**10:00 - 11:00 AM**

**ISEB, Conference Room 5020**

**Abstract:** Ligand-protected gold nanoclusters (AuNCs) are ideal candidates for developing new targeted drug delivery nanosystems with a unique control on their surface functionalities, which can help achieve enhanced delivery performance.

In this work, targeted Au<sub>144</sub> nanoclusters were computationally designed and characterized through extensive classical molecular dynamics (MD) simulations to be potentially employed as combination therapy in gastric cancer treatment. The proposed AuNCs contain cancer cell-recognizing molecules and anticancer drugs on their surface, and we identified the optimal mixed ligand layer to enhance their binding affinity to the cancer cell receptor using atomistic models and enhanced sampling techniques.

The results show that the density of surface ligands is a crucial factor influencing the potential targeting ability of the AuNCs and must be assessed on a case-by-case basis. Our approach demonstrates the potential of carefully controlling the surface composition of AuNCs to optimize their target affinity and specificity, serving as a valuable guide in the experimental phase.

**Bio:** María Francisca Matus is a Senior Researcher in the Nanoscience Center (NSC) at the University of Jyväskylä in the group of Prof. Hannu Häkkinen. She received her Ph.D. in Science in 2018 at the University of Talca (Chile), where her work was focused on the study and characterization of polymeric nanoparticles as drug delivery systems for cardiovascular diseases. Her research focuses on the interface of computational biology and materials science with special emphasis on understanding the interactions between nanoscale materials and biomolecules (nano-bio interface).