

**Materials Day**  
**Abstract Guide**  
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**Spatiotemporal Temperature Control of Nanoparticles via Engineering of Interfacial Heat Transfer and Interfacial Water Properties**

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Noble metal nanoparticles (NPs) are highly efficient in converting light into heat, making them potent nanoscale heat sources. This unique property has been extensively explored in biomedical applications, particularly in photothermal therapy (PTT) and thermally activated drug/gene delivery systems. PTT uses elevated temperatures to destroy cancerous cells (thermolysis), while thermally activated drug delivery systems employ NPs as vehicles where temperature-sensitive chemical linkers control the release of therapeutic agents. Despite their potential, the efficacy of these systems has been limited by off-target reactions due to inefficient temperature control, leading to overdosing and more invasive procedures, which have stalled progress at the preclinical stage. This project aims to conduct a comprehensive investigation into the interfacial heat transfer mechanisms that are critical for deploying engineered noble metal NPs in thermotherapeutics. The project hypothesizes that the overheating problem of NPs can be mitigated by shifting the research focus from the photothermal effect alone to the crucial role of interfacial thermal dissipation, particularly the interfacial chemistry and liquid structuring. In other words, interfacial heat transfer is equally or more important than the photothermal effect in the temperature control of these systems. The research brings together a multidisciplinary team with complementary expertise in metal-water interface modeling, thermal conductance measurement, and spectroscopic analysis of interfacial water properties. The primary objective is to address the longstanding challenge of accurately measuring heat transfer across nanoscale solid-liquid interfaces, thus advancing the development of more effective and safer therapeutic technologies. The approach involves combining experimental techniques, such as spectroscopy and thermorefectance/transmittance, with atomistic computer simulations to engineer the surface chemistry of noble metal NPs for precise cargo-release using temperature-sensitive click-chemistry linkers.