**Computational Catalyst Design for Energy and the Environment**

Giannis Mpourmpakis

Department of Chemical and Petroleum Engineering, University of Pittsburgh, USA

Nanoscale catalysts find tremendous applications in modern industry, facilitating the production of fuels and chemicals, while reducing the energy cost and environmental impact associated with chemical conversion processes. Despite the wide use of catalysts, their application has heavily relied on trial-and-error experimentation in the lab. This lecture will demonstrate how computational research, blending first-principles calculations, multiscale modeling, and machine learning, can help us understand complex catalytic mechanisms, identify active sites on a catalyst surface, design robust, active, and selective catalysts and accelerate catalyst discovery. Examples will include catalysts for thermochemical dehydrogenation of alkanes to olefins, atomically precise electrocatalysts for CO2 reduction, and design of multimetallic nanocatalysts and emergence of single atom alloys. Overall, this seminar will highlight novel rational catalyst design methodologies that help interpret and guide experimentation.