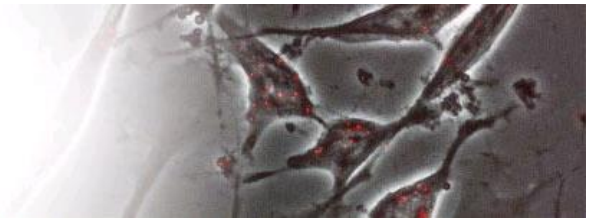
UCLA Engineering

Chemical and Biomolecular Engineering



SEMINARS IN CHEMICAL AND BIOMOLECULAR ENGINEERING

Friday, June 7, 2019
10:00am - 11:00am
Boelter Hall 3400

Thomas Bligaard

Senior Staff Scientist
Chemical Engineering
SLAC National Accelerator Laboratory

"Accelerating catalysis simulations using surrogate machine learning models"

The development of novel catalysts and catalytic processes will be key to mitigating climate change over the next century. Computational atomic-scale simulations holds the promise to help achieving this target. Accelerating simulations of catalytic processes could speed up progress significantly. I will discuss a general framework for accelerating various aspects of atomic-scale catalysis simulations through the application of surrogate machine learning models.

Thomas Bligaard got his education at the Technical University of Denmark, UC Santa Barbara, and the University of Strasbourg. He was a postdoc at the University of Iceland and a faculty member at the Technical University of Denmark before joining SLAC National Accelerator Laboratory, where he is now a Senior Staff Scientist at the SUNCAT Center for Interface Science and Catalysis.