Theoretical Approaches to NanoAlloy Catalysis (WTAC). The WTAC will be a focused meeting of European researchers working in the field of theoretical and computational simulation of catalytic properties and applications of Nanostructured Metal and Metal Oxide Particles, especially in the case of multi- component systems. The workshop will cover the most recent methodological developments in the field of Simulation of Catalysis by NanoAlloys and their practical implementation into computational tools such as software and codes which can be accessed by the community of researchers working in this field.

March 2021	16.	17.	18.	19.
9:00-10:00	Thomas Bligaard, DTU	Karsten Reuter, FHI-MPG	Karoliina Honkala, University of Jyväskylä	Henrik Grönbeck, Chalmers University of Technology
10:30-11:30	Heine A Hansen, DTU	Ivano Castelli, DTU	Jinhyun Chang, DTU	Jan Rossmeisl, University of Copenhagen
12:00-13:00	Break	Break	Break	Break
13:00-16:00	Hands on session 1	Hands on session 2	Hands on session 3	Hands on session 4
16:00-17:00	Zachary Ulissi, Carnegie Mellon University	Andrew A Peterson, Brown University		

Tentative Titles

Thomas Bligaard**:** Machine learning catalysis and fundamentals of catalysis

Heine A Hansen: Workshop introduction and overview

Zachary Ulissi: Machine-learning methods for metal alloy catalysts

Karsten Reuter: Multiscale modeling and machine learning in catalysis research

Ivano Castelli: Big data and computational workflows

Andrew A Peterson: AMP: Atomistic Machine-learning Package

Karoliina Honkala: Zirconia supported rhodium

Jinhyun Chang: CLEASE: CLuster Expansion in Atomic Simulation Environment

Henrik Grönbeck: Computational Catalysis for Metal Nanoparticles

Jan Rossmeisl: High entropy alloy catalysis