



WORKSHOP ON

# TRANSFORMATIONAL MATERIALS II

Addressing the future needs of computing and energy will require radical advances in materials. This workshop will explore the latest theoretical advances in understanding and predicting novel phenomena, such as effects that exhibit extraordinary quantum, electronic, magnetic, optical, topological, or emergent properties, that can lead to transformational materials for computing and energy.

## DAY 1

2:15 pm Introduction

2:30 pm Prof. Frank Ortmann  
Technical University of Munich  
From charge and spin transport to excitons in solar cells: Insights from linear-scaling approaches

3:30 pm Prof. Kristian Sommer Thygesen  
Technical University of Denmark  
High-throughput modeling and discovery of atomically thin crystals

4:30 pm Coffee Break

5:00 pm Prof. André Schleife  
U of Illinois at Urbana-Champaign  
Triggering ion dynamics in materials by laser and particle radiation

6:00 pm Prof. Evan Reed  
Stanford University  
Syntheziable yet unsynthesized low-dimensional materials revealed by data science

## DAY 2

2:15 pm Introduction

2:30 pm Prof. Michele Ceriotti  
EPFL  
Physics-inspired machine learning for molecular and materials modeling

3:30 pm Prof. Aleksandra Vojvodic  
University of Pennsylvania  
Modeling chemistry of compound materials for catalysis and energy

4:30 pm Coffee Break

5:00 pm Prof. Kristin Persson  
University of California at Berkeley  
The era of data-driven materials innovation and design

6:00 pm Wrap-Up

OCT. 7, 2021:  
2:15 PM - 7:00 PM

OCT. 8, 2021:  
2:15 PM - 6:15 PM

ONLINE

