

Workshop: Materials Data Science for Accelerating Materials Discovery and Design

March 22nd – March 23rd, 2021

Organisers

Christoph Brabec (FAU Erlangen, Germany)
Ralf Drautz (RUB, Germany)
Alfred Ludwig (RUB, Germany)
Markus Stricker (RUB, Germany)
Ichiro Takeuchi (University of Maryland, USA)

Program

March 22nd, 2021

Time (CET)	Speaker	Title
3:00 p.m. - 3:10 p.m.		WELCOME
3:10 p.m. - 3:40 p.m.	Sergei Kalinin <i>Oak Ridge National Laboratory, USA</i>	“Physical generative models from the imaging data: toward materials prediction and design.”
3:40 p.m. - 4:10 p.m.	Maria K. Chan <i>Argonne National Laboratory, USA</i>	“Combining computational modeling and machine learning for characterization data inversion.”
4:10 p.m. - 4:40 p.m.	Phil Maffetone <i>Brookhaven National Laboratory, USA</i>	“Artificial intelligence powered beamline science for remote, on-the-fly materials analysis.”
4:40 p.m. - 5:00 p.m.	Lars Banko <i>Ruhr-University Bochum, Germany</i>	“Predictive structure zone diagrams.”
5:00 p.m. - 5:10 p.m.	BREAK	
5:10 p.m. - 5:40 p.m.	Raymundo Arroyave <i>Texas A&M University, USA</i>	“Multi Information Fusion Bayesian Optimization of Materials.”
5:40 p.m. - 6:10 p.m.	Ralf Rettig <i>Thermo-Calc Software AB, Stockholm, Sweden</i>	“Strategies and approaches for flexible integration of simulation tools in ICME.”
6:10 p.m. - 6:30 p.m.	Setareh Zomorodpoosh <i>Ruhr-University Bochum, Germany</i>	“Application of artificial intelligence to design of novel superalloys.”

6:30 - 6:40 p.m.	BREAK	
6:40 p.m. - 7:10 p.m.	Kenneth S. Vecchio <i>University of California San Diego, USA</i>	“Machine Learning Enabled High-throughput Rapid Experimental Alloy Development.”
7:10 p.m. - 7:30 p.m.	Pascal Thome <i>Ruhr-University Bochum, Germany</i>	“Digital Microscopy: Optimization, Microstructure Characterization and Machine Learning.”
7:30 p.m. - 8:00 p.m.	DISCUSSION	

March 23rd, 2021

Time (CET)	Speaker	Title
3:00 p.m. - 3:30 p.m.	Chris Wolverton <i>Northwestern University, USA</i>	“Network Theory Meets Materials Science.”
3:30 p.m. - 4:00 p.m.	Bryce Meredig <i>Citrine Informatics, USA</i>	“Delivering materials informatics capabilities to industry.”
4:00 p.m. - 4:20 p.m.	Thomas Hammerschmidt <i>Ruhr-University Bochum, Germany</i>	“Machine-learning materials with domain-knowledge from electronic-structure coarse-graining.”
4:40 p.m. - 5:00 p.m.	Yury Lysogorskiy <i>Ruhr-University Bochum, Germany</i>	“Data-driven platform for atomistic modelling and simulations.”
5:00 p.m. - 5:10 p.m.	BREAK	
5:10 p.m. - 5:30 p.m.	Aaron Gilad Kusne <i>National Institute of Standards and Technology, USA</i>	“Autonomous Materials Research and Discovery at NIST.”
5:30 p.m. - 6:00 p.m.	Elsa Olivetti <i>Massachusetts Institute of Technology, USA</i>	“Bridging the Gap Between Literature Data Extraction and Domain Specific Materials Informatics.”
6:00 p.m. - 6:20 p.m.	Helge Stein <i>Karlsruhe Institute of Technology & Helmholtz Institute Ulm, Germany</i>	“Materials acceleration platforms for energy storage and production.”
6:20 p.m. - 6:40 p.m.	Gero Egels <i>Ruhr-University Bochum, Germany</i>	“A computational approach to the microstructural design of high-speed steels.”
6:40 p.m. - 7:00 p.m.	Pascal Friederich <i>Karlsruhe Institute of Technology, Germany</i>	“Machine Learning as a tool to accelerate and scale up atomistic materials simulations.”
7:00 p.m. - 7:15 p.m.	BREAK	
7:15 p.m. - 8:00 p.m.	DISCUSSION	
END OF MEETING		