

## Symposium Big data driven materials science (SYBD)

jointly organized by  
the Metal and Material Physics Division (MM),  
the Surface Science Division (O), and  
the Chemical and Polymer Physics Division (CPP)

Jörg Neugebauer  
MPI für Eisenforschung  
Max-Planck-Str. 1  
40237 Düsseldorf  
neugebauer@mpie.de

Matthias Scheffler  
Fritz-Haber-Institut der MPG  
Faradayweg 6  
14195 Berlin  
scheffler@fhi-berlin.mpg.de

Kurt Kremer  
MPI für Polymerforschung  
Ackermannweg 10  
55021 Mainz  
kremer@mpip-mainz.mpg.de

Combining concepts from big data analytics with experimental and theoretical techniques in solid state physics has opened exciting new routes to designing materials with superior mechanical, electronic or optical properties as well as to enhance resolution and performance of established experimental techniques as e.g. electron microscopy, x-ray diffraction, or atom probe tomography. The symposium will bring together leading experts who pioneer the application of these techniques for their respective fields. The intention is to show success stories but also to critically discuss present limitations as well as emerging areas. A critical aspect that will be in the focus of the symposium is that big data analytics alone, i.e. without a deep understanding of the underlying physics, turns out to be insufficient in successfully addressing experiment or materials related challenges.

Topics to be addressed in the symposium are: exploring high-dimensional chemical, crystallographic and microstructural compound spaces by big data analytics; linking physical, chemical, and mechanical theories with materials data platforms across scales; pushing resolution limits of atomic-scale and meso-scale experimental techniques in microscopy, spectroscopy, and tomography; applications ranging from structural materials surviving extreme conditions to soft matter and solid-state surfaces.

## Overview of Invited Talks and Sessions

(Lecture hall HSZ 02)

### Invited Talks

SYBD 1.1	Tue	9:30–10:00	HSZ 02	<b>Materials innovation driven by data and knowledge systems</b> — •SURYA KALIDINDI
SYBD 1.2	Tue	10:00–10:30	HSZ 02	<b>Network Theory Meets Materials Science</b> — •CHRIS WOLVERTON, MURAT AYKOL, VINAY HEGDE
SYBD 1.3	Tue	10:30–11:00	HSZ 02	<b>Verification and error estimates for ab initio data</b> — •CLAUDIA DRAXL
SYBD 1.4	Tue	11:15–11:45	HSZ 02	<b>Identifying Domains of Applicability of Machine Learning Models for Materials Science</b> — •MARIO BOLEY, CHRISTOPHER SUTTON, LUCA M. GHIRINGHELLI, MATTHIAS RUPP, JILLES VREEKEN, MATTHIAS SCHEFFLER
SYBD 1.5	Tue	11:45–12:15	HSZ 02	<b>Deep learning of low-dimensional latent space molecular simulators</b> — •ANDREW FERGUSON

### Sessions

SYBD 1.1–1.5	Tue	9:30–12:15	HSZ 02	<b>Big Data Driven Materials Science</b>
--------------	-----	------------	--------	--