From Physics and Big Data to the Design of Novel Materials (SYNM)

jointly organised by the Metal and Material Physics Division (MM), the Chemical and Polymer Physics Division (CPP), the Semiconductor Physics Division (HL), and the Thin Films Division (DS)

Jörg Neugebauer	Matthias Scheffler	Kurt Kremer
Max-Planck-Institut für	Fritz-Haber-Institut der	Max-Planck-Institut für
Eisenforschung	Max-Planck-Gesellschaft	Polymerforschung
Düsseldorf	Berlin	Mainz
neugebauer@mpie.de	scheffler@fhi-berlin.mpg.de	${\rm kremer@mpip-mainz.mpg.de}$

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.

Overview of Invited Talks and Sessions

(Lecture hall H1)

Invited Talks

SYNM 1.1	Mon	15:00 - 15:30	H1	How to tackle the "I" in FAIR? — •CLAUDIA DRAXL
SYNM 1.2	Mon	15:30 - 16:00	H1	Beyond the average error: machine learning for the discovery of novel
				materials — •Mario Boley, Simon Teshuva, Felix Luong, Lucas Foppa,
				Matthias Scheffler
SYNM 1.3	Mon	16:00-16:30	H1	The Phase Diagram of All Inorganic Materials — • CHRIS WOLVERTON
SYNM 1.4	Mon	16:45 - 17:15	H1	Automated data-driven upscaling of transport properties in materials
				— •Danny Perez, Thomas Swinburne
SYNM 1.5	Mon	17:15-17:45	H1	Data-driven understanding of concentrated electrolytes — \bullet ALPHA LEE

Sessions

SYNM 1.1-1.5 Mc	on 15:00–17:45	H1	From Physics and Big D	Data to the Design of Nov	vel Materials
-----------------	----------------	----	------------------------	---------------------------	---------------