

Big Data Summer – Program

Monday, September 9, 2019

15:00	Arrival – Coffee break	
Session chair: Claudia Draxl		
15:30 - 16:30	Matthias Scheffler	Welcome and Introduction
16:30 - 17:30	Jilles Vreeken	Material Subgroups
17:30 - 18:00	Break	
18:00 - 19:00	Hans-Joachim Bungartz	Research Data Infrastructures – How Generic can & should they be?
19:30	Welcome Cocktail - Dinner	

Tuesday, September 10, 2019

08:00	Breakfast	
Session chair: Hans-Joachim Bungartz		
09:00 - 10:00	Claudia Draxl	The NOMAD Encyclopedia – a Tool for Exploring Computed Data
10:00 - 11:00	Dierk Raabe	Big Data-Related Challenges in Microstructure Research and Alloy Design
11:00 - 11:30	Break	
11:30 - 12:30	Siyuan Zhang	Modern Electron Microscopy goes high Dimension: Handling Big Data
12:30 - 12:50	Hot Topic Talk: Raabe (Atomic-Scale Imaging of Chemistry at Lattice Defects)	
13:00 - 15:00	Lunch Break	
Session chair: Matthias Scheffler		
15:00 - 16:00	Joseph F. Rudzinski	Data-Driven Methods for Soft Matter
16:00 - 16:20	Hot Topic Talk: Vreeken (Telling Cause from Effect)	
16:20 - 16:50	Break	
16:50 - 20:00	Poster Parade and Poster Session	
20:00	Dinner	

Wednesday, September 11, 2019

08:00	Breakfast	
Session chair: Isao Tanaka		
09:00 - 09:45	Markus Rampp	High-Performance Data Analytics: Basic Concepts of Distributed Deep Learning
09:45 - 10:45	Karsten W. Jacobsen	Machine Learning and Computational Screening
10:45 - 11:15	Break	
11:15 - 12:15	Luca M. Ghiringhelli	Metadata Towards FAIR Data Sharing for Data-Driven Materials Science
12:15 - 12:55	Hot Topic Talks: <ul style="list-style-type: none"> - Jacobsen (High Entropy Alloys for Catalysis) - Draxl (Benchmark Calculations Towards Ultimate Precision in Density-Functional Theory) 	

13:00 - 15:00	Lunch break	
<i>Session chair: Karsten W. Jacobsen</i>		
15:00 - 16:00	Cécile Hébert	<i>Data Challenges in Analytical Transmission Electron Microscopy: Size, Formats and Annotation</i>
16:00 - 16:40	Hot Topic Talks: <ul style="list-style-type: none"> - Ghiringhelli (Identifying Interpretable Descriptors for Materials Properties with Subgroup Discovery and Information Theory) - Rudzinski (Variational Autoencoders for Dimensionality Reduction and Clustering of Molecular Dynamics Data) 	
16:40 - 17:20	Break	
17:20 - 18:20	Annette Trunschke	<i>Big-Data Driven Catalysis Research: Challenges and Chances</i>
18:20 - 18:40	Hot Topic Talk: Hébert (Machine Learning Techniques in Analytical TEM: Trends and Challenges)	
20:00	Dinner	

Thursday, September 12, 2019

08:00	Breakfast	
<i>Session chair: Stefan Bauer</i>		
09:00 - 10:00	Chiho Kim	<i>Polymer Informatics: Past, Present, and Future</i>
10:00 - 10:40	Hot Topic Talks: <ul style="list-style-type: none"> - Bauer (Learning Disentangled Representations) - Tanaka (Data Driven Discovery of New Materials) 	
10:40 - 11:10	Break	
11:10 - 12:10	Luca M. Ghiringhelli	<i>Learning Descriptors for Materials Properties with Symbolic Regression and Compressed Sensing</i>
12:10 - 12:30	Hot Topic Talk: Trunschke (Clean Data Acquisition in Oxidation Catalysis)	
13:00	Lunch break	
14:30	Excursion and Conference Dinner	

Friday, September 13, 2019

8:00	Breakfast	
<i>Session chair: Matthias Scheffler</i>		
09:00 - 10:00	Stefan Bauer	<i>Recent Advances in Unsupervised Representation Learning</i>
10:00 - 11:00	Isao Tanaka	<i>Recommender System for Materials Discovery</i>
11:00	Concluding remarks	