

International Workshop
15th - 18th April 2019

BiGmax Workshop 2019 on Big-data-driven Materials Science

PROGRAM



Scientific coordinators:

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Organisation:

Maria Voigt



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The program will be continuously updated during the event. This
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Program

Monday, 15 April

08:00 - 16:30	<i>Registration in guest house 4, library</i>
11:00 - 12:00	Informal discussions
12:00 - 13:00	Lunch break
13:00 - 14:00	Informal discussions
14:00 - 15:30	Tutorial I - Introduction to Deep Learning
15:30 - 16:00	Coffee break
16:00 - 17:30	Tutorial II - Introduction to Compressed Sensing
17:30 - 18:00	Discussions
18:00 - 19:30	Welcome dinner
19:30 - 20:30	Informal discussions

Tuesday, 16 April

- 09:30 - 09:40 **Jan Michael Rost (MPIPKS),
Peter Benner & Matthias Scheffler**
Opening
- 09:40 - 10:00 **BiGmax scientific advisor on
software engineering Markus Kühbach**
(Max-Planck-Institut für Eisenforschung Düsseldorf)

Chair morning talks: Markus Rampp
- 10:00 - 10:30 **Kailash Budhathoki** (Max-Planck-Institut für
Informatik Saarbrücken)
Rule Discovery for Exploratory Causal Reasoning
- 10:30 - 11:00 Coffee break
- 11:00 - 11:30 **Christoph Freysoldt** (Max-Planck-Institut für
Eisenforschung Düsseldorf)
Automatic feature detection in STEM data sets
by unsupervised learning
- 11:30 - 12:00 **Luca Ghiringhelli** (Fritz-Haber-Institut der
Max-Planck-Gesellschaft Berlin)
Compressed Sensing for data-driven materials
science
- 12:00 - 13:00 Lunch break
- 13:00 - 15:00 PI Meeting

Chair afternoon talk: Tristan Bereau

- 15:00 - 16:00 **Anatole von Lilienfeld** (Universität Basel)
Quantum Exploration of Chemical Space
- 16:00 - 18:00 Poster session
- 18:00 - 19:00 Dinner
- 19:00 - 20:00 Informal discussions

Wednesday, 17 April

Chair morning talks: Ulf Saalman

- 09:00 - 10:00 **Alpha Lee** (University of Cambridge)
Data-driven chemical discovery: Making sense of noisy and limited data
- 10:00 - 10:10 **Group photo**
(to be published on the event's web page)
- 10:10 - 10:30 Coffee break
- 10:30 - 11:00 **Benedikt Hoock** (Fritz-Haber-Institut der Max-Planck-Gesellschaft & Humboldt-Universität Berlin)
Feature construction and selection towards optimal descriptors for materials properties
- 11:00 - 11:30 **Markus Kühbach** (Max-Planck-Institut für Eisenforschung Düsseldorf)
Materials Science Examples for Structural Characterizing of Point Cloud Data at Scale
- 11:30 - 12:00 **Markus Rampp** (Max-Planck-Gesellschaft - Computing and Data Facility)
A new machine learning cluster at the MPCDF
- 12:00 - 13:00 Lunch break
- 13:00 - 14:00 Discussions

Chair afternoon talks: Christopher Sutton

- 14:00 - 14:30 **Benjamin Regler** (Fritz-Haber-Institut der Max-Planck-Gesellschaft Berlin)
Discovering functional relationships between atomic and materials properties: an information-theoretic machine learning approach
- 14:30 - 15:00 **Leigh Stephenson**
(Max-Planck-Institut für Eisenforschung Düsseldorf)
Big-data-enabled true analytical atomic-scale tomography
- 15:00 - 15:30 **Paolino De Falco** (Max-Planck-Institut für Kolloid- und Grenzflächenforschung Potsdam)
3D SAXS Tomography
- 15:30 - 16:00 Coffee break
- 16:00 - 16:30 **Markus Scheidgen** (Fritz-Haber-Institut der Max-Planck-Gesellschaft & Humboldt-Universität Berlin)
FAIR experimental material science data with NOMAD
- 16:30 - 17:00 **Ye Wei**
(Max-Planck-Institut für Eisenforschung Düsseldorf)
Deploying machine learning for information extraction from atom probe datasets
- 17:00 - 17:30 **Arghya Dutta**
(Max-Planck-Institut für Polymerforschung Mainz)
Application of data mining techniques in soft matter systems
- 17:30 - 18:00 Discussions

Program

- 18:15 Departure to the Neustadt of Dresden by tram from the institute (meeting point: reception of MPIPKS)
- 19:00 - 21:00 Conference dinner at the restaurant and pub **Bautzner Tor**
Hoyerswerdaer Straße 37, 01099 Dresden
Tel.: +49 351 8038202

Thursday, 18 April

Chair talks: Leigh Stephenson

- 09:00 - 09:30 **Christopher Sutton** (Fritz-Haber-Institut der Max-Planck-Gesellschaft Berlin)
The NOMAD 2018 Kaggle Competition:
Tackling Materials-Science Challenges through Crowd Sourcing
- 09:30 - 10:00 **Kiran Kanekal**
(Max-Planck-Institut für Polymerforschung Mainz)
Quantifying the reduction of chemical compound space due to coarse-graining
- 10:00 - 10:30 Coffee break
- 10:30 - 11:00 **Ulf Saalman** (Max-Planck-Institut für Physik komplexer Systeme Dresden)
Disentangle photo-electron spectra from fluctuating pulses
- 11:00 - 11:30 **Santiago Rigamonti** (Humboldt-Universität Berlin)
CELL: a python package for cluster expansion with a focus on complex alloys
- 11:30 - 12:00 **Peter Benner & Matthias Scheffler**
Concluding remarks
- 12:00 - 13:00 Lunch break
- 13:00 - 15:00 Discussions & departure