BiGmax Workshop 2019 on Big-Data-Driven Materials Science

MPI Dresden

15th – 18th April 2019

Scientific Organizers: Tristan Bereau (MPI Mainz), Jan Michael Rost (MPI Dresden)

Local Organizer: Maria Voigt (MPI Dresden)

Contents

Scope of the workshop

Materials science is entering an era where the growth of data from experiments and calculations is expanding beyond a level that is properly processable by established scientific methods. Dealing with this big data is not just a technical challenge, but much more: it offers great opportunities. Big-data analytics will revolutionize new material discovery and will make the successful search of structure-property relationships among multiple length and time scales possible.

Summary of the events

The workshop this year helped bring the experimentalists with the theoreticians closer together. We have seen a lot more interactions between members, as well as a common language and framework shaping up throughout the talks, suggesting more coherence in the network. Smaller discussion rounds focused around technical topics helped students and postdocs exchange more intensively. The invited talks were regarded very positively as inspiring research directions. Overall we've received positive feedback from various members of the network.

Discussed Topics

- Structure and plasticity of materials
- Data diagnostics in 3D imaging
- Discovering interpretable patterns, correlations, and causality
- Learning thermodynamic properties of materials
- Materials Encyclopedia (incl. metadata for experimental samples and methods)

Invited speakers

- Alpha Lee (UK)
- Anatole von Lilienfeld (CH)

Program

April 15th, 2019

08:00 - 16:30	Registration in guest house 4, library
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

April 16th, 2019

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

April 17th, 2019

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
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

April 18th, 2019

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 Saalmann** (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

Speakers abstracts

- **Kailash Budhathoki** (Max-Planck-Institut für Informatik Saarbrücken), *Rule Discovery for Exploratory Causal Reasoning*

Traditional descriptive rule discovery techniques struggle with the consistent detection of (potentially rare) events that have a strong effect on some output variable. The sources of inconsistency are two-fold: Firstly, naive empirical effect estimations have a high variance, and, hence, their maximization is highly optimistically biased unless the search is artificially restricted to high-frequency events. Secondly, actual effect sizes are often skewed by the presence of confounding factors, which is a concern, especially in scientific data analysis. To address both these issues, we present a novel descriptive rule discovery approach based on reliably estimating the conditional effect given the value of potential confounders. We demonstrate that the corresponding score is a conservative and consistent effect estimator and derive an efficient optimization algorithm that successfully detects valuable rules on a multitude of real datasets. Importantly, the presented approach allows for a natural iterative rule discovery where new non-redundant rules can be found by treating previously discovered rules as confounders in subsequent iterations.

- **Christoph Freysoldt** (Max-Planck-Institut für Eisenforschung Düsseldorf), *Automatic feature detection in STEM data sets by unsupervised learning*

Scanning transmission electron microscopy (STEM) is an essential tool in material science to understand the microstructure of complex materials such as steels. In STEM, a focused electron beam scans over a thin sample in a 2D grid. Multiple detectors are available to collect the scattered electrons in various directions as well as optical excitations induced. Modern instrumentation even allows to repeat the experiment on the same location in rapid succession, giving a temporal dimension to the data. In consequence, STEM provides huge multi-dimensional multi-channel data sets that encode the crystallographic and chemical microstructure of the sample, and possibly its temporal evolution. We aim at developing a set of tools to explore the scientific content of STEM data, i.e. identify in a semi-automatic way the crystalline phases, grain boundaries, dislocations etc. I will explain our strategy for unsupervised automatic segmentation in the x-y scanning plane as a crucial first step. It is based on exploring spatial correlations in the high-angle annular dark-field detector channel that reflect the underlying crystal lattice. I will show our current achievements.

- **Luca Ghiringhelli** (Fritz-Haber-Institut der Max-Planck-Gesellschaft Berlin), *Compressed Sensing for data-driven materials science*

The number of possible materials is practically infinite, while only few hundred thousands of (inorganic) materials are known to exist and for few of them even basic properties are systematically known. In order to speed up the identification and design of new and novel optimal materials for a desired property or process, strategies for quick and well-guided exploration of the materials space are highly needed. A desirable strategy would be to start from a large body of experimental or theoretical data, and by means of artificial-intelligence methods, to identify yet unseen patterns or structures in the data. This leads to the identification of maps (or charts) of materials where different regions correspond to materials with different properties. The main challenge on building such maps is to find the appropriate descriptive parameters (called descriptors) that define these regions of interest. Here, I will present methods for the machine-aided identification of descriptors and materials maps applied to the metal/insulator classification, the prediction of novel topological insulators, and of carbon-dioxide activation on metal-oxide surfaces.

- **Anatole von Lilienfeld** (Universität Basel), *Quantum Exploration of Chemical Space*

Many of the most relevant chemical properties of matter depend explicitly on atomistic and electronic details, rendering a first principles approach to chemistry mandatory. Alas, even when using high-performance computers, brute force high-throughput screening of compounds is beyond any capacity for all but the simplest systems and properties due to the combinatorial nature of chemical space, i.e. all compositional, constitutional, and conformational isomers. Consequently, efficient exploration algorithms need to exploit all implicit redundancies present in chemical space. I will discuss recently developed statistical learning and computational alchemy based approaches for rigorously yet efficiently estimating quantum mechanical observables in compositional and constitutional space. Results for our models indicate remarkable performance in terms of accuracy, speed, universality, and size scalability.

- **Alpha Lee** (University of Cambridge), *Data-driven chemical discovery: Making sense of noisy and limited data*

Although significant progress has been made in combining machine learning with theoretical calculations, translating machine learning predictions to experimentally-confirmed materials is still a significant challenge. What is often overlooked is that experimental chemistry and materials science are expensive, time-consuming and the data is not necessarily noise-free. This has two important consequences: First, datasets of experimentally-measured properties are often quite small. Second, a robust estimation of model uncertainty is needed to gauge the "risk" versus "return" of experimentally verifying a particular prediction. I will discuss our recent work on developing uncertainty-calibrated model with noisy and limited data in the context of drug discovery. The mathematics of random matrices, as well as Bayesian statistics and statistical physics, all come to our rescue. We have developed experimentally-validated models that suggest novel and potent organic molecules against therapeutically relevant receptors, as well as ways to chemically synthesise those novel molecules. I will also discuss how insights from drug discovery can be translated into materials science problems.

- **Benedikt Hoock** (Fritz-Haber-Institut der Max-Planck-Gesellschaft & Humboldt-Universität Berlin), *Feature construction and selection towards optimal descriptors for materials properties*

Materials data contained in repositories like NOMAD [1] can be exploited in many useful ways, such as to better understand existing materials or to discover new materials with desired properties. A crucial step towards these goals is to find a set of meaningful descriptors, i.e. parameters based on computationally cheap input data that capture the physical mechanisms underlying certain material properties. In this work, we develop principles for constructing up to millions of candidate descriptors from simple physical properties. These principles involve mathematical operations [2] and different averaging procedures considering the local ordering. We compare two compressed sensing methods, LASSO+l0 [2] and SISSO [3], at identifying optimal descriptors out of all the candidates. Likewise, we introduce and compare cross-validation based model-selection strategies that use either the average training or the average test error as a criterion, aiming at increasing the descriptors' generalizability. We use two ab initio data sets, comprising group-IV zincblende ternaries and transparent conducting oxides, to test this methodological approaches. [1]: C. Draxl & M. Scheffler, MRS Bulletin, 43, 676 (2018). [2]: L. M. Ghiringhelli, et. al., Phys. Rev. Lett. 114, 105503 (2015). [3]: R. Ouyang, et. al., Phys. Rev. Mater. 2, 083802 (2018).

- **Markus Kühbach** (Max-Planck-Institut für Eisenforschung Düsseldorf), *Materials Science Examples for Structural Characterizing of Point Cloud Data at Scale*

Distilling knowledge from output of ever larger getting experimental characterization or full-field simulation output demands frequently to handle point clouds with associated mark data. I will present recent examples from processing Atom Probe Tomography and full-field annealing microstructure evolution simulations which detail how the Materials scientist can economize its knowledge extraction process by making rigorous use of High Performance Computing paradigms.

- **Markus Rampp** (Max-Planck-Gesellschaft - Computing and Data Facility), *A new machine learning cluster at the MPCDF*

The groups of M. Scheffler, K. Kremer, D. Raabe, and J. Neugebauer, in collaboration with the MPCDF have designed and procured a dedicated machine-learning compute cluster which is operated by MPCDF (as of early 2019) and which will be open for collaborations arising in BiGmax. The talk will provide a brief overview of the cluster configuration (hardware and software environment), basic usage and first experiences with machine-learning applications.

- **Benjamin Regler** (Fritz-Haber-Institut der Max-Planck-Gesellschaft Berlin), *Discovering functional relationships between atomic and materials properties: an information-theoretic machine learning approach*

Machine learning predictively maps features to target properties without providing insights why some features are more relevant than others. However, an identification of feature relevance does not only lead to useful knowledge about unknown outcomes but also improves the performance of learning algorithms. By means of feature selection and information theory, we quantify the relevance of features via estimating information shared between features and target properties. More specifically, we aim to identify relationships between fundamental properties at the atomistic scale and materials properties at the macroscopic scale. We perform comparisons with existing feature selection methods and explore potential issues of our design. Further, we highlight our approach on case studies and present first materials science applications, namely octet-binary compound semiconductors and predicting compressive strength of concrete. Eventually, we conclude that information-theoretic feature selection is a viable tool to explain feature relevance and to pre-process scientific data for machine-learning tasks.

- **Leigh Stephenson** (Max-Planck-Institut für Eisenforschung Düsseldorf), *Big-data-enabled true analytical atomic-scale tomography*

Field ion microscopy (FIM) provides a magnified image of a cryogenically-cooled, needle-like specimen subjected to a high electric field [1]. Projected gas ions form an image in which a specimen's surface atoms can be individually observed. A three dimensional variant of FIM (3DFIM) stimulates incremental field evaporation of surface atoms so that a FIM image sequence can be converted into a 3D atomic reconstruction [2]. While 3DFIM can resolve both a crystalline lattice and its structural defects (such as vacancies and dislocations), the use of existing 3DFIM techniques are largely hampered by the enormous computational costs associated with acquiring and storing large quantities of image data and subsequently performing the required feature analysis and reconstruction. Its potential has been unexploited for two other reasons. Modern FIM techniques have been spurned in preference to atom probe tomography (APT), a technique that while giving lower spatial resolution otherwise provides invaluable time-of-flight spectrometry that allows the chemical identification of atoms. Secondary to this, few modern commercial atom probes have FIM capabilities and there are only a few bespoke FIM machines. Preliminary work at MPIE (performed

jointly between the atom probe group and the computational department) has demonstrated that FIM-equipped atom probes can operate in a hybrid pulsed FIM/APT mode for a varied materials applications. The resulting tof-FIM data is rich with nanostructural information, and can be processed to resemble APT point cloud data or transformed to a versatile 3DFIM representation. Significantly, we demonstrated that our atom probes are sufficiently able to perform time-of-flight mass spectrometry in the presence of an imaging gas without compromising instrument integrity and, furthermore, a signal from field evaporated specimen atoms can be easily differentiated from the field ionised imaging signal. Here we present the first steps of a collaboration between MPIE, MPI for Intelligent Systems (MPIIS) and the Max Planck Computing and Data Facility (MPCDF). Some of the experimental aspects will be mentioned, but the focus will be on the early challenges of inferring missing information and intelligently turning "bad" data into "good" data for the use of predictive methods.

- **Paolino De Falco** (Max-Planck-Institut für Kolloid- und Grenzflächenforschung Potsdam), *3D SAXS Tomography*

The structural complexity of biological materials requires new methodology of material characterization in three and even four dimensions including time. We explore new 3D imaging methods based on x-ray scattering using synchrotron sources that can provide important information on the nanostructure of materials. In a tomography experiment at a synchrotron source data collection requires several hours. Consequently, the size of relevant data produced by this new approach tremendously grows resulting also in an increasing need of computational power and time for 3D reconstruction of data. The focus of our research is the development of a new methodology for fast characterizations of the 3D nanostructure of bone. On the nanoscopic length scale bone is a composite of a fibrous collagen matrix in which inorganic calcium phosphate particles are incorporated. The mineral particles decisively contribute to the high mechanical stiffness and strength of bone material. We aim to elucidate the 3D distribution of mineral particle sizes within a certain bone volume, which is a relevant parameter to characterize the influence of bone diseases on the bone's mechanical properties. We present results from our approach based on SAXS (small angle X-ray scattering) tomography experiments collected at synchrotron sources and mathematical algorithms of image reconstruction.

- **Markus Scheidgen** (Fritz-Haber-Institut der Max-Planck-Gesellschaft & Humboldt-Universität Berlin), *FAIR experimental material science data with NOMAD*

The NOMAD (Novel Material Discovery) Center of Excellence (http://nomad-coe.eu) developed the world's largest platform for sharing computational material science data over the past years. NOMAD integrates heterogenous data from many computational material science codes and allows to Find Access Interoperate and Reuse (FAIR) data through a common (meta)data format. The experimental material science community faces similar challenges when trying to share data from various experimental methods, hardware, and labs. In this talk, we look at the first steps in opening the NOMAD platform for experimental material science data.

- **Ye Wei** (Max-Planck-Institut für Eisenforschung Düsseldorf), *Deploying machine learning for information extraction from atom probe datasets*

In this work, we explore data extraction in atom probe tomography utilizing machine learning technique. First, we applied unsupervised learning to atom probe datasets from a Zr-Al- Cu-Fe bulk metallic glass (BMG) in both an undeformed and a deformed state to detect amorphous nanospheres. More specially, we implemented a clustering analysis using Hierarchical Density-Based Spatial Clustering of Applications with Noise (HDBSCAN). Second, assigning an elemental identity of

peaks or deconvolute peak overlaps in the mass spectrum is a critical step to perform accurate microanalysis by atom probe and measure a precise chemical composition. This has been so far largely performed by human expertise, which is time-consuming and often marred by manual errors. Therefore, we propose a new automatic approach to perform with assistance of machine learning (mean-shift clutering and gradient boosted decision trees). Ye Wei, Ebrahim Norouzi ,Micheal Herbig, Shanoob Balachandran Nair, Baptiste Gault, Dierk Raabe (Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany)

- **Arghya Dutta** (Max-Planck-Institut für Polymerforschung Mainz), *Application of data mining techniques in soft matter systems*

Data mining helps in finding, and predicting, materials showing some desired property using statistical methods. It becomes very useful when the subset of materials showing the property becomes small or the pattern becomes too intricate for relatively easy modeling. In this talk, I will present results from our recent and ongoing work on how data mining can provide useful insights for complex soft matter systems.

- **Christopher Sutton** (Fritz-Haber-Institut der Max-Planck-Gesellschaft Berlin), The NOMAD 2018 Kaggle Competition: Tackling Materials-Science Challenges through Crowd Sourcing

Machine learning (ML) promises to accelerate the discovery of novel materials by screening candidate compounds at signicantly lower computational cost than traditional electronic-structure approaches. However, it is often a priori unclear which ML models are suitable for a given problem and optimizing a model can be a time-consuming endeavor. Crowd sourcing allows for comparing several ML models by identifying a key problem and challenging the community to solve it. To this end, the Novel Materials Discovery (NOMAD) Centre of Excellence together with Kaggle one of the most well-known hosting platforms - organized an open data-science competition to predict two key properties of transparent conducting oxides (TCOs): band gap energy (for transparency) and formation energy (for stability). Although these materials are crucial for optoelectronic devices, only a small number TCOs are currently known. In this contribution, we present the winning model out of nearly 900 participants based on a novel crystal-graph representation and an analysis of the relative importance of representation vs regression model for the performance of several ML approaches.

- **Kiran Kanekal** (Max-Planck-Institut für Polymerforschung Mainz), Quantifying the reduction of chemical compound space due to coarse-graining

In an in silico search for structure-property relationships, the extensive computational resources required by atomistic molecular dynamics simulations renders a thorough exploration of chemical compound space unfeasible. This issue can be efficiently addressed by relying on coarse-grained models, which provide a means to mitigate the computational expense while still capturing the relevant physical properties of the system under investigation. In this work, we introduce a high-throughput screening of chemical compound space by means of coarse-grained molecular dynamics simulations of the Martini force field, and apply it to the determination of the insertion thermodynamics of an ensemble of small molecules in a phospholipid bilayer environment [1]. We show that Martini, as a chemically transferable coarse-grained model, yields a significant reduction in the size of chemical space. However, the Martini model is not optimal for chemical transferability, and we next propose new criteria for the rational design of coarse-grained models that allows for the optimization of their chemical transferability. We validate this hypothesis by parameterizing three Martini-like force fields, in which the number of bead types ranges from five to sixteen for the different force fields. We demonstrate that a level of performance and accuracy comparable to Martini can be obtained by using a force field with fewer bead types, thus making this force field more efficient at reducing the chemical compound space. Furthermore, constructing this force field

with chemical transferability as a foundation allows us to know a priori the most likely chemistries that correspond to a specific bead type. [1] R. Menichetti, K.H. Kanekal, and T. Bereau, ACS Cent. Sci. 5(2), (2019).

- **Ulf Saalmann** (Max-Planck-Institut für Physik komplexer Systeme Dresden), Disentangle photo-electron spectra from fluctuating pulses

Conventional free-electron laser machines create strongly fluctuating pulses that change from shot to shot. Non-linear processes driven by those pulses depend critically on the actual fluctuation pattern, which is typically not of genuine interest. Here we discuss an attempt to "straighten" those pulses a posteriori. By means of artificial neural networks we map photo-electron spectra from fluctuating pulses to those from idealized ones.

- **Santiago Rigamonti** (Humboldt-Universität Berlin), CELL: a python package for cluster expansion with a focus on complex alloys

We present the python package CELL, which allows for building accurate cluster expansion (CE) models of materials. A wide variety of substitutional systems can be treated with CELL, including one, two, and three-dimensional materials, as well as multi-component and multi-lattice systems. Most notably, it is capable of dealing with complex materials containing several (>30) atoms in their parent lattice. It uses state-of-the art techniques for model selection and finite-temperature simulations. The power of the code is illustrated by a number of examples ranging from simple (e.g. a Si-Ge alloy) to more involved workflows (e.g. an iterative CE construction for a clathrate alloy) built with the provided interface. CELL also provides a bash command line interface, visualization utilities, and can be interfaced with virtually all ab-initio codes.

Poster contribution

- First-Principles Thermodynamics of ZrO2 at Hybrid-DFT Level Using a Machine-Learned Potential. **Ahmetcik, Emre**
- Screening of small molecules with bilayer-modifying properties using coarse-grained simulations. **Centi, Alessia**
- Convolutional Neural Networks for Near-field Spectroscopy. **Eisfeld, Alexander**
- Denoising photoelectron spectra using autoencoder. **Giri, Sajal Kumar**
- Predicting solute-grain boundary segregation energies. **Huber, Liam**
- Structure-selection strategies in the cluster-expansion method. **Hübner, Axel**
- Toward Generalised Subgroup Discovery. **Kalofolias, Giannis**
- Nonlinear classification: A Kernelized Support Tensor Train Machine. **Kour, Kirandeep**
- Towards an Accurate, High-throughput Framework for the Prediction of Anharmonic Free Energies in Molecular Crystals: Benchmarks. **Krynski, Marcin**
- A framework for studying similarity: Recommending materials in the NOMAD Encyclopedia. **Kuban, Martin**
- Robust crystal-structure recognition using Bayesian deep learning. **Leitherer, Andreas**
- Machine Learning of Free Energies. **Rauer, Clemens**
- Machine Learning for Multidimensional Photoemission Spectroscopy. **Stimper, Vincent**
- Temperature-dependent properties of thermoelectric clathrates. **Troppenz, Maria**

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