BiGmax Virtual ML Workshop June, 15th and 16th 2020

Speakers:

- We have two sessions. Check your respective slot in the program below.
- All talks are to be given as a live talk using screen share followed by questions.
- The time for all talks is given in Central European Time (CET).
- **We expect that all speakers enter the stream in due time before their talk to allow for a smooth transition between the talks. Thank you very much.**
- The sessions will be recorded. The recordings will be shared on the BiGmax/MaxNet intranet.

Posters:

- **Posters will be presented via live screen share in a poster pitch followed by questions.** The poster pitch is a 3min free talk where the poster presenters can guide the viewers through the essential findings of their poster. Thereafter, the audience can ask questions. The posters should be prepared as PDFs. We understand that these posters may show newest results. Therefore, sharing the PDF document - beyond presenting it in the meeting - is recommended but not mandatory.

How to tune in?

- **Links to the video conference channel will be communicated Friday, (12th) afternoon.**
- Feel free to drop any specific questions you have at **bigmaxml2020@mpie.de**.

We wish you all the best for you and your families and would like to welcome you very much to participate actively in this virtual BiGmax meeting on data-driven Materials Science

Markus Kühbach (on behalf of the organization team),
Dierk Raabe,
Jörg Neugebauer,
Gerhard Dehm,
Christoph Freysoldt,
Baptiste Gault,
Christian Liebscher,
Michael Ashton

Topic 1: June, 15th 2020, session starting at 2pm

*Challenges and critical problems when using ML/AI image processing methods to reconstruct the geometry and properties of crystal defects from microscopy data (**Moderator:** Markus Kühbach)*

Talks:

S1, 20min **Sandra Korte-Kerzel** (invited), Institut für Metallkunde und Metallphysik, RWTH Aachen
Combining high resolution and large area imaging with deep learning –
A new tool to understand damage in dual phase microstructures
S1 10min Q/A

S2, 12min **Ning Wang**, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf
Automatic semantic segmentation of Scanning Transmission Electron Microscopy (STEM) images using an unsupervised machine learning approach
S2, 8min Q/A

S3, 12min **Byung Chul Yeo**, Fritz-Haber-Institut, Berlin
Automatic Identification of Crystallographic Surfaces from Scanning Transmission Electron Microscopy Dataset by Artificial Intelligence
S3, 8min Q/A

S4, 12min **Ye Wei**, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf
A data-driven approach towards predicting mechanical properties of advanced steel
S4, 8min Q/A

S5, 12min **Astrid Perlade**, ArcelorMittal Global R&D, Maizières-lès-Metz Cedex
Digital product development initiatives at ArcelorMittal
S5, 8min Q/A

S6, 12min **Luca Bertinetti**, Max-Planck-Institut für Kolloid und Grenzfl., Potsdam/Golm
Deep Learning for 3D segmentation of big bioimaging datasets
S6, 8min Q/A Intermediate time: 2h 10min

Poster pitches:

P1, 3min **Pawan Goyal**, Max-Planck-Institut für Dynamik komplexer technischer Systeme, Magdeburg
3D SAXS tomography to determine spatial heterogeneities in the nano-structure of bovine bone

P2, 3min **Sedareh Medghalchi**, Institut für Metallkunde und Metallphysik, RWTH Aachen
Large-area, high-resolution characterisation and classification of damage mechanisms in dual-phase steel using deep learning

P3, 3min **Niels Cautaerts**, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf
TEM data, metadata and the sample description problem

P4, 3min **Steffen Brinckmann**, Forschungszentrum Jülich, IEK-2, Jülich
#tbd poster on TEM metadata

P5, 3min **Xuyang Zhou**, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf
Automated grain boundary detection via a convolutional neural network to assist in-plane composition mapping in atom probe tomography

P6, 3min **Yue Li**, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf
Revealing ordered structure in Al-Mg-Li alloys by combining machine learning and atom probe tomography

P123456, 32min Q/A + pointing at slack channels Total time: 3h

Topic 2: Tuesday, June 16th 2020, 9am

Challenges and critical problems for efficiency and uncertainty quantification of ML/AI used in ab-initio methods.
*(**Moderation:** #tbd)*

Talks:

S7, 20min **Alexander Shapeev** (invited), Skoltech, Moscow
Seamless acceleration of ab initio materials modeling with machine learning
S7, 10min Q/A

S8, 12min **Daniel Speckhard**, Fritz-Haber-Institut, Berlin
Error Estimation of Energy per Atom of Semiconductor Compounds Using Statistical Learning
S8, 8min Q/A

S9, 12min **Thomas Purcell**, Fritz-Haber-Institut, Berlin
Uncovering Anharmonicity in Material Space
S9, 8min Q/A

S10, 12min **Lucas Foppa**, Fritz-Haber-Institut, Berlin
Hierarchical SISSO: predicting complex materials properties building on simpler ones
S10, 8min Q/A

S11, 12min **Mariana Rossi**, Fritz-Haber-Institut, Berlin
In silico Characterisation of Vibrational Properties of Molecular Crystals
S11, 8min Q/A

S12, 12min **Marcin Krynski**, Fritz-Haber-Institut, Berlin
Transferable Gaussian Process Regression for prediction of molecular crystals harmonic free energy
S12, 8min Q/A

S13, 12min **Vincent Stimper**, Max-Planck-Institut für Intelligente Systeme, Tübingen
#tbd
S13, 8min Q/A

Total time: 2h 30min

Poster pitches:

P7, 3min **Andreas Leitherer**, Fritz-Haber-Institut, Berlin
Versatile Bayesian deep-learning framework for crystal-structure recognition
in single- and polycrystalline materials

P8, 3min **Andrea Cacioppo**, Max-Planck-Institut für Intelligente Systeme, Tübingen
Deep Learning for Tight-Binding Hamiltonians

P78, 30min Q/A + pointing at slack channels

Total time: 3h