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Narodowe Centrum Badań Jądrowych  
National Centre for Nuclear Research  
SWIERK

Organizers:



Centre of Excellence in Multifunctional Materials  
for Industrial and Medical Applications

# 1st NOMATEN International Conference on Materials Informatics

Wednesday 01 June 2022 - Friday 03 June 2022

NCBJ HQ in Otwock / Hybrid Mode

## Scientific Program (last updated: May 30<sup>th</sup>, 2022)

June 1<sup>st</sup>

### Welcome Session

- Welcome Address: NCBJ Director prof. Krzysztof Kurek (10:00-10:05)
- Welcome Address: Atomic energy and Materials Science in Poland (Ministry of Climate and Environment) (10:05-10:10)
  - NAWA Welcome Address 1 (Mr Piotr Kępski) (10:10-10:20)
- Welcome Address: Christophe Galle (CEA, Partner of NOMATEN CoE) (10:20-10:25)
- NOMATEN Center of Excellence and Research Goals: Mikko Alava (NOMATEN CoE Director) (10:25-10:30)  
[coffee break] (10:30-10:45)
- Overview of the Conference Programme (Stefanos Papanikolaou) (10:45-11:00)

### Plenary Presentation:

11:00-11:50: Surya Kalidindi, Georgia Tech, USA,  
Machine Learning and Materials Informatics Innovation: Current State  
[Lunch Buffet] (12:00 - 13:00)

### Session 1: Mechanics and defects in crystals: Large data and machine learning (13:00 - 15:15)

Chair: Fabrizio Rovaris (NCBJ)

- 13:00 - 13:45: Michael Zaiser (FAU Erlangen, Germany), *\*online, Machine learning microstructure-property relations in mechanics of materials: Prediction, Diagnosis, Optimization.*
- 13:45 - 14:15: Silvia Bonfanti (NCBJ, Poland), *Predicting the failure of two-dimensional silica glasses.*
- 14:15 - 14:45: Javier Dominguez (NCBJ, Poland), *Machine learning based atomistic dislocation modeling of nanoindentation of irradiated crystalline materials.*
- 14:45 - 15:15: Juha Koivisto (Aalto U, Finland), *Thermal gelation of cellulosic fiber methylcellulose mixtures: rheological phases using Bayesian optimization.*

[coffee break] [15:15 - 15:30]

### Session 2: Interatomic Potentials towards proper capture of mesoscale effects in molecular simulations (15:30 - 18:15)

Chair: Lasse Laurson (Tampere U)

- 15:30 - 16:15 : Boris Kozinsky (Harvard University, USA), *Symmetry and uncertainty-aware machine learning models of atomic interactions and dynamics.*
- 16:15 - 17:00 : M. Cosmin Marinica (CEA, France), *Machine Learning for Atomistic Materials Science*
- 17:00 - 17:45 : Gabriel Stoltz (ENPC, France), *Coarse-graining molecular systems with autoencoders and adaptive sampling.*
- 17:45 - 18:15 : Jan Wrobel (Warsaw University of Technology, Poland), *Modelling of properties of Ta-Ti-V-W high-entropy alloys using DFT-based machine learning potentials.*

[Poster Session & Buffet] [18:15 - 19:30]

June 2<sup>nd</sup>

[Breakfast at Hotel -- Buses leave at ~07:45]

### Session 3: Large Data Mechanics and Physics of Solids: Applications of materials informatics (09:00-12:15) Chair: Silvia Bonfanti (NCBJ)

- 09:00 - 09:45: Udo von Toussaint (MPI, Plasmaphysics, Munich, Germany), *Physics inspired Machine Learning (ML) Approaches for Materials Science: On the importance of representations, prior information and adaptive.*

09:45 - 10:15 : Stephanie C. TerMaath (U. Tennessee, USA), *Reduced order modeling to characterize the damage tolerance of metal/composite hybrid structure.*

10:15 - 10:45: Thomas Hochrainer (TU Graz, Austria), *Characterizing discrete dislocation configurations with alignment tensors and correlations.*

10:45 - 11:15: Lasse Laurson (Tampere U, Finland), *Inferring Microstructure-Property Relationships in Discrete Dislocation Plasticity: Deformation Predictability and Materials Design.*

11:15 - 11:45: Luca Messina (CEA, France), *Atomic-scale modeling of chemically disordered compounds by means of generative models.*

11:45 - 12:15: Henri Salmenjoki (Aalto U, Finland), *Correlation between dislocation avalanches and the impact on the stress-strain curve.*

[Lunch Buffet] (12:15 - 12:45)

Session 4. Material discovery, materials by design and Multiscale Materials Modeling (12:45-15:00)

Chair: Javier Dominguez (NCBJ)

12:45 - 13:30: Y. Morris Wang (UCLA, USA), *Critical modelling and informatics need for materials in additive manufacturing*

13:30 - 14:00: Milica Todorovic (Uturk U, Finland), *Computational materials engineering with active learning*

14:00 - 14:30: Noel Jakse (Grenoble, France), *Crystal nucleation in metallic systems: Unsupervised topological learning approach.*

14:30 - 15:00 Thomas Swinburn (CINaM, Luminy, Aix-Marseille University, France), *Data-driven models for plasticity and thermodynamics in discrete and continuous state spaces.*

[coffee break] [15:00-15:15]

Session 5. Machine Learning, Ontologies and data operability approaches in a FAIR world (15:15-18:00)

Chair: Amin Esfandiarpour (NCBJ)

15:15 - 16:00: Stefan Sandfeld (FZ Jülich, Germany) \*online, *From Ontologies and FAIR Data to Machine Learning-based High-Throughput Data Mining of In-Situ TEM Experiments on Dislocations in HEAs*

16:00 - 16:45: Wing-Kam Liu (Northwestern U, USA) \*online, *Hierarchical Deep Learning Neural Network (HiDeNN)-FEM-AI for process design and performance prediction of material systems.*

16:45 - 17:30: Maciej Mazurowski (Duke U, USA) \*online, *Deep learning in medical imaging*

17:30 - 18:00: Akhtar Zeb (VTT, Finland), *Ontological modelling of creep void analysis data to automate machine learning training process.*

[Welcome Dinner -- Restauracja Warszawska -- Warsaw Downtown -- 20:15]

June 3<sup>rd</sup>

Session 6. Industry applications and opportunities of materials informatics methods (09:30-12:15)

Chair: Karol Frydrych (NCBJ)

09:30 - 10:15 : Arkadiusz Sitek (Sano Institute, Poland), *Sano Centre for Computational Medicine - journey to transform healthcare.*

10:15 - 10:45 : Pawel Sobkowicz (NCBJ, Poland), *Selected legal aspects of AI/ML development and deployment.*

10:45 - 11:15 : Anna Wawrzynczak-Szaban (NCBJ, Poland), *The Artificial Neural Network Model for the contamination source emergency localization system.*

11:15 - 11:45 : Kamran Karimi (NCBJ), *Using machine learning to predict short-range ordering in metallic glasses.*

11:45 - 12:15 : Marcin Minkowski (TAU, Finland), *Strain-rate-dependent predictability of discrete dislocation plasticity.*

[Lunch Buffet] (12:15 - 12:45)

Concluding Remarks Round Table (June 3<sup>rd</sup>) (12:45 - 13:15)