Conference Programme

August 31th, 2023
Convention Centre, Ruhr-Universität Bochum

8:30 – 9:00 a.m.	Registration
9:00 – 9:10 a.m.	**Ralf Drautz** (Ruhr-Universität Bochum, Germany): Welcome on behalf of the Materials Chain, room 2a
Session 1	**Data-driven Materials Science**
9:10 – 9:40 a.m.	**Walid Hetaba** (Max-Planck-Institut für Chemische Energiekonversion, Germany): "FAIR research data infrastructure and its importance for data driven materials science – the role of FAIRmat."
9:40 – 10:10 a.m.	**Tilmann Hickel** (Bundesanstalt für Materialforschung und -prüfung, Germany): "Research data infrastructures as enablers for materials design."
10:10 – 10:30 a.m.	Coffee Break
Session 2	**Materials Informatics in Industry**
10:30 – 11:00 a.m.	**James Saal** (Citrine Informatics, USA): "Closed-loop materials design with artificial intelligence."
11:00 – 11:30 a.m.	**Michele Matsuo, Mauricio Santaella** (Otto Fuchs, Germany): "Employing machine learning methods in an industry context at Otto Fuchs KG."
11:30 – 12:00 p.m.	**Moritz to Baben** (GTT-Technologies, Germany): "Materials informatics for phase stability simulations."
12:00 – 1:30 p.m.	Postersession with snacks and cold drinks, room 1
Session 3	**Materials Informatics for Simulations**
1:30 – 2:00 p.m.	**Karin Everschor-Sitte** (Universität Duisburg-Essen, Germany): "In-materio reservoir computing based on magnetic skyrmions."
2:00 – 2:30 p.m.	**Jörg Behler** (Ruhr-Universität Bochum, Germany): "Four generations of neural network potentials."
2:30 – 3:00 p.m.	**Johannes Margraf** (Fritz-Haber-Institut, Germany): "Science-driven chemical machine learning."
3:00 – 3:20 p.m.	Coffee Break
Session 4	**Materials Informatics for Experiments**
3:20 – 3:50 p.m.	**Baptiste Gault** (Max-Planck-Institut für Eisenforschung, Germany): "Integrating machine-learning in atom probe tomography analysis workflows."
3:50 – 4:20 p.m.	**Christoph Freysoldt** (Max-Planck-Institut für Eisenforschung, Germany): "Perspectives for machine-learning applied to data-rich experiments on complex materials."
4:20 – 4:40 p.m.	Coffee Break
Session 5	**Research Data Management**
4:40 – 5:10 p.m.	**Patrick Lambrix** (Linköping University, Sweden): "Semantic access to materials databases using the materials design ontology."
5:10 – 5:40 p.m.	**Johannes Frenzel, Andreas Schramm** (Ruhr-Universität Bochum, Germany): "Making data management feel easy – Integration of a data repository into the research process."
5:40 – 5:50 p.m.	**Markus Stricker** (Ruhr-Universität Bochum, Germany): Closing remarks