MCIC 2021: Materials Discovery and Processing for Energy

November 22nd, 2021

Conference programme

9:00 – 9:10 a.m.	**Welcome**
Session 1	**Materials for physical energy conversion, 2D and hybrid functional materials**
9:10 – 9:40 a.m.	**Christoph Brabec** (FAU Erlangen-Nürnberg, Germany): "Accelerating perovskites: towards stable composites and solar cell devices"
9:40 – 10:10 a.m.	**Jonathan Finley** (TU Munich, Germany): "Hex-SiGe: A new direct bandgap semiconductor"
10:10 – 10:30 p.m.	**Gerd Bacher** (University of Duisburg-Essen, Germany): "(MO)CVD grown 2D materials for scalable optoelectronic devices"
Session 2	**Materials for chemical energy conversion**
10:30 – 10:50 a.m.	**Sven Reichenberger** (University of Duisburg-Essen, Germany): "Laser-generated multinary high entropy alloy nanoparticles for catalytical applications"
10:50 – 11:20 a.m.	**Mehtap Oezaslan** (TU Braunschweig, Germany): "Platinum-based alloy electrocatalysts for hydrogen oxidation reaction (HOR) and oxygen reduction reaction (ORR)"
11:20 – 11:50 a.m.	**Marc Koper** (Leiden U, The Netherlands): "New views on the electrochemistry of platinum"
11:50 – 12:30 p.m.	Break
Session 3	**Magnetic materials for energy conversion**
12:30 – 1:00 p.m.	**Oliver Gutfleisch** (TU Darmstadt, Germany): "Hysteresis design of magnetic materials for efficient energy conversion"
1:00 – 1:20 p.m.	**Anna Grünebohm** (Ruhr-Universität Bochum, Germany): "Hysteresis design of ferroelectric materials"
1:20 – 1:40 p.m.	**Karin Everschor-Sitte** (University of Duisburg-Essen, Germany): "Towards energy efficient magnetic in materio computing"
1:40 – 2:00 p.m.	**Anna Böhmer** (Ruhr-Universität Bochum, Germany): "Caloric effects in correlated materials"
2:00 – 2:20 p.m.	Break
Session 4	**Metals and Alloys**
2:20 – 2:50 p.m.	**Dierk Raabe** (MPIE): "Reduction of iron oxides with hydrogen: pathways towards sustainable metallurgy"
2:50 – 3:20 p.m.	**Jannica Heinrichs** (Uppsala U, Sweden): "Tool wear and surface modifications in metal machining"
3:20 – 3:40 p.m.	**Stefanie Hanke** (University of Duisburg-Essen, Germany): "Microstructural damage mechanisms in metals exposed to cavitation"
3:40 – 4:00 p.m.	Break
Session 5	**Production engineering and additive manufacturing**
4:00 – 4:30 p.m.	**Stefanie Reese** (RWTH Aachen, Germany): "Efficient multi-scale modeling by means of FE-FFT and model order reduction techniques"
4:30 – 5:00 p.m.	**Katrin Wudy** (TU Munich, Germany): "New process strategies for laser-based powder bed fusion of metals"
5:00 – 5:20 p.m.	**Ulf Apfel** (Ruhr-Universität Bochum, Germany): "From catalysts to high performance electrodes: from fundamental to applied research in electrolysis"

Session 6	Data-driven and combinatorial materials discovery
5:20 – 5:50 p.m.	**Gus Hart** (Brigham Young University, USA): “Building useful MLIPs”
5:50 – 6:20 p.m.	**John Gregoire** (Caltech, USA): “High throughput discovery of solar fuels materials”
6:20 – 6:40 p.m.	**Markus Stricker** (Ruhr-Universität Bochum, Germany): "Machine learning for plasticity"
6:40 – 7:30 p.m.	**Final Discussion**
7:30 p.m.	**End of Conference**