

## Metal and Material Physics Division Fachverband Metall- und Materialphysik (MM)

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### Overview of Invited Talks and Sessions

(Lecture rooms H 0106, H 0107, TC 006, and TC 010; Poster C and E )

#### Invited Talks

|         |     |             |        |                                                                                                                                                                                                                              |
|---------|-----|-------------|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| MM 1.1  | Mon | 9:30–10:00  | TC 006 | <b>Beyond Hall-Petch: Mechanism based description of dislocation grain-boundary interactions</b> — ●CHRISTOPH KIRCHLECHNER, NATALIYA MALYAR, JUAN LI, NICOLAS PETER, CHRISTIAN LIEBSCHER, JEAN-SEBASTIEN MICHA, GERHARD DEHM |
| MM 9.1  | Mon | 15:00–15:30 | TC 006 | <b>Deciphering fracture patterns: what crack paths teach us about the mechanics and physics of fracture</b> — ●LAURENT PONSON                                                                                                |
| MM 18.1 | Tue | 9:30–10:00  | TC 006 | <b>Hydrogen storage in individual metal nanoparticles</b> — ●ANDREA BALDI, TARUN NARAYAN, FARIAH HAYEE, AI LEEN KOH, ROBERT SINCLAIR, JENNIFER DIONNE                                                                        |
| MM 28.1 | Wed | 9:30–10:00  | TC 006 | <b>Accurate and fast machine learning n-body force fields</b> — ALDO GLIELMO, CLAUDIO ZENI, JAMES KERMODE, ●ALESSANDRO DE VITA                                                                                               |
| MM 49.1 | Thu | 9:30–10:00  | TC 006 | <b>Analysis of amorphous structures by transmission electron microscopy</b> — ●MARTIN PETERLECHNER                                                                                                                           |
| MM 59.1 | Thu | 15:00–15:30 | TC 006 | <b>Dilatometric Techniques for Atomic Scale Analysis of Defects and Processes in Solids</b> — ●WOLFGANG SPRENGEL                                                                                                             |

#### Invited talks of the joint symposium SYID

See SYID for the full program of the symposium.

|          |     |             |        |                                                                                                                                          |
|----------|-----|-------------|--------|------------------------------------------------------------------------------------------------------------------------------------------|
| SYID 1.1 | Mon | 9:30–10:00  | H 0105 | <b>Data driven R&amp;D for Materials: Cognitive Discovery</b> — ●ALESSANDRO CURIONI                                                      |
| SYID 1.2 | Mon | 10:00–10:30 | H 0105 | <b>Rational design and synthesis of Pt-based catalysts for fuel cell applications</b> — ●YOUNAN XIA                                      |
| SYID 1.3 | Mon | 10:30–11:00 | H 0105 | <b>2D, or not 2D? Materials discovery, data provenance, and workflow reproducibility.</b> — ●NICOLA MARZARI                              |
| SYID 1.4 | Mon | 11:00–11:30 | H 0105 | <b>Generating and assessing data from combinatorial and high-throughput experiments for the design of new materials</b> — ●ALFRED LUDWIG |
| SYID 1.5 | Mon | 11:30–12:00 | H 0105 | <b>Novel materials discovery: big-data-analytics methods and infrastructure for building maps of materials</b> — ●LUCA GHIRINGHELLI      |

#### Invited talks of the joint symposium SYMS

See SYMS for the full program of the symposium.

|          |     |             |        |                                                                                                                            |
|----------|-----|-------------|--------|----------------------------------------------------------------------------------------------------------------------------|
| SYMS 1.1 | Mon | 15:00–15:30 | H 0105 | <b>Stochastic numerical algorithms: from molecular dynamics to big data analytics</b> — ●BENEDICT LEIMKUHLER               |
| SYMS 1.2 | Mon | 15:30–16:00 | H 0105 | <b>A Generally-Applicable Machine-Learning Scheme for Materials and Molecules</b> — ●MICHELE CERIOTTI                      |
| SYMS 1.3 | Mon | 16:00–16:30 | H 0105 | <b>Girsanov reweighting for path ensembles and Markov state models</b> — ●BETTINA G. KELLER, LUCA DONATI, CARSTEN HARTMANN |

|          |     |             |        |                                                                                                  |
|----------|-----|-------------|--------|--------------------------------------------------------------------------------------------------|
| SYMS 1.4 | Mon | 16:45–17:15 | H 0105 | <b>Liquid State Theory Meets Deep Learning and Molecular Informatics</b> — ●ALPHA LEE            |
| SYMS 1.5 | Mon | 17:15–17:45 | H 0105 | <b>Computational high-throughput screening of drug-membrane thermodynamics</b> — ●TRISTAN BEREAU |

### Invited talks of the joint symposium SYDM

See SYDM for the full program of the symposium.

|          |     |             |        |                                                                                                                           |
|----------|-----|-------------|--------|---------------------------------------------------------------------------------------------------------------------------|
| SYDM 1.1 | Thu | 15:00–15:30 | H 0105 | <b>Bending, pulling, and cutting wrinkled two-dimensional materials</b> — ●KIRILL BOLOTIN                                 |
| SYDM 1.2 | Thu | 15:30–16:00 | H 0105 | <b>Ultrafast valley and spin dynamics in single-layer transition metal dichalcogenides</b> — ●ALEJANDRO MOLINA-SANCHEZ    |
| SYDM 1.3 | Thu | 16:00–16:30 | H 0105 | <b>Interlayer excitons in layered semiconductor transition metal dichalcogenides</b> — ●STEFFEN MICHAELIS DE VASCONCELLOS |
| SYDM 1.4 | Thu | 16:45–17:15 | H 0105 | <b>Exploring exciton physics in liquid-exfoliated 2D materials</b> — ●CLAUDIA BACKES                                      |
| SYDM 1.5 | Thu | 17:15–17:45 | H 0105 | <b>A Progress Report on Electron Transport in MXenes; A New Family of 2D Materials</b> — ●MICHEL BARSOUM                  |

### Invited talks of the joint symposium SYAM

See SYAM for the full program of the symposium.

|          |     |             |        |                                                                                                                                |
|----------|-----|-------------|--------|--------------------------------------------------------------------------------------------------------------------------------|
| SYAM 1.1 | Fri | 9:30–10:00  | H 0105 | <b>Bringing Dino-Birds to life – Synchrotron X-ray fluorescence and Raman imaging of ancient materials</b> — ●UWE BERGMANN     |
| SYAM 1.2 | Fri | 10:00–10:30 | H 0105 | <b>Linear and Nonlinear Optical Properties of Cultural Heritage Materials</b> — ●MARTA CASTILLEJO                              |
| SYAM 1.3 | Fri | 10:30–11:00 | H 0105 | <b>Morphology and topology of multiscale pore networks: Imaging structural alteration and hydric invasion</b> — ●PIERRE LEVITZ |
| SYAM 1.4 | Fri | 11:15–11:45 | H 0105 | <b>Painting cracks: a way to reveal physical properties of matter</b> — ●LUDOVIC PAUCHARD                                      |
| SYAM 1.5 | Fri | 11:45–12:15 | H 0105 | <b>Finite element analysis and biomechanical interpretation of fossil material properties</b> — ●EMILY RAYFIELD                |

### Sessions

|              |     |             |        |                                                                                                                                                                  |
|--------------|-----|-------------|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| MM 1.1–1.1   | Mon | 9:30–10:00  | TC 006 | <b>Invited talk Kirchlechner</b>                                                                                                                                 |
| MM 2.1–2.5   | Mon | 10:15–11:30 | H 0106 | <b>Battery Materials</b>                                                                                                                                         |
| MM 3.1–3.8   | Mon | 10:15–13:15 | H 0107 | <b>Topical session (Symposium MM): Hydrogen in Materials</b>                                                                                                     |
| MM 4.1–4.4   | Mon | 10:15–11:30 | TC 006 | <b>Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales</b>                                                                             |
| MM 5.1–5.8   | Mon | 10:15–13:15 | TC 010 | <b>Topical session (Symposium EPS and MM, joint session with MA): Magnetism in Materials Science: Thermodynamics, Kinetics and Defects (joint session MM/MA)</b> |
| MM 6.1–6.10  | Mon | 10:30–13:00 | HL 001 | <b>Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials I (joint session O/MM/DS/TT/CPP)</b>                                   |
| MM 7.1–7.5   | Mon | 11:45–13:00 | H 0106 | <b>Battery Materials</b>                                                                                                                                         |
| MM 8.1–8.5   | Mon | 11:45–13:15 | TC 006 | <b>Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales</b>                                                                             |
| MM 9.1–9.1   | Mon | 15:00–15:30 | TC 006 | <b>Invited talk Ponson</b>                                                                                                                                       |
| MM 10.1–10.5 | Mon | 15:45–17:00 | H 0106 | <b>Battery Materials</b>                                                                                                                                         |
| MM 11.1–11.3 | Mon | 15:45–17:00 | H 0107 | <b>Topical session (Symposium MM): Hydrogen in Materials</b>                                                                                                     |
| MM 12.1–12.5 | Mon | 15:45–17:15 | TC 006 | <b>Topical Session (Symposium MM): Fundamentals of Fracture</b>                                                                                                  |
| MM 13.1–13.8 | Mon | 15:45–18:45 | TC 010 | <b>Topical session (Symposium EPS and MM, joint session with MA): Magnetism in Materials Science: Thermodynamics, Kinetics and Defects (joint session MM/MA)</b> |
| MM 14.1–14.9 | Mon | 15:00–17:15 | HL 001 | <b>Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials II (joint session O/MM/DS/TT/CPP)</b>                                  |

|               |     |             |          |                                                                                                                                                                  |
|---------------|-----|-------------|----------|------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| MM 15.1–15.5  | Mon | 17:30–18:45 | H 0106   | <b>Battery Materials</b>                                                                                                                                         |
| MM 16.1–16.5  | Mon | 17:30–19:00 | H 0107   | <b>Topical session (Symposium MM): Hydrogen in Materials</b>                                                                                                     |
| MM 17.1–17.5  | Mon | 17:30–19:00 | TC 006   | <b>Topical Session (Symposium MM): Fundamentals of Fracture</b>                                                                                                  |
| MM 18.1–18.1  | Tue | 9:30–10:00  | TC 006   | <b>Invited talk Baldi</b>                                                                                                                                        |
| MM 19.1–19.5  | Tue | 10:15–11:30 | H 0106   | <b>Battery Materials</b>                                                                                                                                         |
| MM 20.1–20.8  | Tue | 10:15–13:00 | H 0107   | <b>Topical session (Symposium MM): Hydrogen in Materials</b>                                                                                                     |
| MM 21.1–21.4  | Tue | 10:15–11:30 | TC 006   | <b>Topical Session (Symposium MM): Fundamentals of Fracture</b>                                                                                                  |
| MM 22.1–22.4  | Tue | 10:15–11:15 | TC 010   | <b>Microstructure and Phase Transformations</b>                                                                                                                  |
| MM 23.1–23.5  | Tue | 10:30–13:00 | HL 001   | <b>Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials III (joint session O/MM/DS/TT/CPP)</b>                                 |
| MM 24.1–24.4  | Tue | 11:45–13:00 | H 0106   | <b>Topical session (Symposium EPS and MM, joint session with MA): Magnetism in Materials Science: Thermodynamics, Kinetics and Defects (joint session MM/MA)</b> |
| MM 25.1–25.6  | Tue | 11:45–13:15 | TC 006   | <b>Topical Session (Symposium MM): Fundamentals of Fracture</b>                                                                                                  |
| MM 26.1–26.5  | Tue | 11:45–13:00 | TC 010   | <b>Microstructure and Phase Transformations</b>                                                                                                                  |
| MM 27.1–27.34 | Tue | 18:30–19:45 | Poster E | <b>Poster Session I</b>                                                                                                                                          |
| MM 28.1–28.1  | Wed | 9:30–10:00  | TC 006   | <b>Invited talk De Vita</b>                                                                                                                                      |
| MM 29.1–29.4  | Wed | 10:15–11:15 | H 0106   | <b>Nanomaterials</b>                                                                                                                                             |
| MM 30.1–30.5  | Wed | 10:15–11:30 | H 0107   | <b>Interfaces</b>                                                                                                                                                |
| MM 31.1–31.4  | Wed | 10:15–11:30 | TC 006   | <b>Topical session (Symposium MM): Fundamentals of Fracture</b>                                                                                                  |
| MM 32.1–32.4  | Wed | 10:15–11:15 | TC 010   | <b>Microstructure and Phase Transformations</b>                                                                                                                  |
| MM 33.1–33.9  | Wed | 10:30–13:00 | HL 001   | <b>Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials IV (joint session O/MM/DS/TT/CPP)</b>                                  |
| MM 34.1–34.4  | Wed | 11:45–12:45 | H 0106   | <b>Nanomaterials</b>                                                                                                                                             |
| MM 35.1–35.5  | Wed | 11:45–13:00 | H 0107   | <b>Interfaces</b>                                                                                                                                                |
| MM 36.1–36.5  | Wed | 11:45–13:00 | TC 006   | <b>Topical Session (Symposium MM): Fundamentals of Fracture</b>                                                                                                  |
| MM 37.1–37.5  | Wed | 11:45–13:00 | TC 010   | <b>Microstructure and Phase Transformations</b>                                                                                                                  |
| MM 38.1–38.4  | Wed | 15:15–16:15 | H 0106   | <b>Nanomaterials</b>                                                                                                                                             |
| MM 39.1–39.6  | Wed | 15:15–16:45 | H 0107   | <b>Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales</b>                                                                             |
| MM 40.1–40.5  | Wed | 15:15–16:45 | TC 006   | <b>Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century</b>                              |
| MM 41.1–41.6  | Wed | 15:15–16:45 | TC 010   | <b>Liquid and Amorphous Metals</b>                                                                                                                               |
| MM 42.1–42.10 | Wed | 15:00–17:45 | HL 001   | <b>Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials V (joint session O/MM/DS/TT/CPP)</b>                                   |
| MM 43.1–43.4  | Wed | 17:00–18:00 | H 0106   | <b>Nanomaterials</b>                                                                                                                                             |
| MM 44.1–44.4  | Wed | 17:00–18:15 | H 0107   | <b>Topical Session (Symposium EPS and MM): Mechanical Properties at Small Scales</b>                                                                             |
| MM 45.1–45.5  | Wed | 17:00–18:30 | TC 006   | <b>Topical Session (Symposium MM): Fundamentals of Fracture</b>                                                                                                  |
| MM 46.1–46.6  | Wed | 17:00–18:30 | TC 010   | <b>Liquid and Amorphous Metals</b>                                                                                                                               |
| MM 47.1–47.51 | Wed | 18:30–19:45 | Poster C | <b>Poster Session II</b>                                                                                                                                         |
| MM 48         | Wed | 19:45–20:45 | TC 006   | <b>General Assembly of the Metal- and Materials Division</b>                                                                                                     |
| MM 49.1–49.1  | Thu | 9:30–10:00  | TC 006   | <b>Invited talk Peterlechner</b>                                                                                                                                 |
| MM 50.1–50.4  | Thu | 10:15–11:30 | H 0106   | <b>Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales</b>                                                                             |
| MM 51.1–51.6  | Thu | 10:15–11:45 | H 0107   | <b>Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century</b>                              |
| MM 52.1–52.5  | Thu | 10:15–11:30 | TC 006   | <b>Methods in Computational Materials Modelling (methodological aspecst, numerics)</b>                                                                           |
| MM 53.1–53.5  | Thu | 10:15–11:30 | TC 010   | <b>Liquid and Amorphous Metals</b>                                                                                                                               |
| MM 54.1–54.9  | Thu | 10:30–12:45 | HL 001   | <b>Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VI (joint session O/MM/DS/TT/CPP)</b>                                  |
| MM 55.1–55.4  | Thu | 11:45–13:00 | H 0106   | <b>Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales</b>                                                                             |

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|---------------|-----|-------------|--------|-------------------------------------------------------------------------------------------------------------------------------------|
| MM 56.1–56.5  | Thu | 11:45–13:15 | H 0107 | <b>Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century</b> |
| MM 57.1–57.6  | Thu | 11:45–13:15 | TC 006 | <b>Methods in Computational Materials Modelling (methodological aspect, numerics)</b>                                               |
| MM 58.1–58.6  | Thu | 11:45–13:15 | TC 010 | <b>Liquid and Amorphous Metals</b>                                                                                                  |
| MM 59.1–59.1  | Thu | 15:00–15:30 | TC 006 | <b>Invited talk Sprengel</b>                                                                                                        |
| MM 60.1–60.3  | Thu | 15:45–16:45 | H 0106 | <b>Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales</b>                                                |
| MM 61.1–61.5  | Thu | 15:45–17:15 | H 0107 | <b>Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century</b> |
| MM 62.1–62.6  | Thu | 15:45–17:15 | TC 006 | <b>Methods in Computational Materials Modelling (methodological aspect, numerics)</b>                                               |
| MM 63.1–63.5  | Thu | 15:45–17:00 | TC 010 | <b>Transport (Diffusion, conductivity, heat)</b>                                                                                    |
| MM 64.1–64.10 | Thu | 15:00–17:45 | HL 001 | <b>Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VII (joint session O/TT/MM/DS/CPP)</b>    |
| MM 65.1–65.6  | Thu | 17:30–19:00 | H 0106 | <b>Functional Materials (Actuators, filters, sensors, shape memory)</b>                                                             |
| MM 66.1–66.5  | Thu | 17:30–19:00 | H 0107 | <b>Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century</b> |
| MM 67.1–67.6  | Thu | 17:30–19:00 | TC 006 | <b>Methods in Computational Materials Modelling (methodological aspect, numerics)</b>                                               |
| MM 68.1–68.4  | Thu | 17:30–18:30 | TC 010 | <b>Transport (Diffusion, conductivity, heat)</b>                                                                                    |
| MM 69.1–69.5  | Fri | 9:30–10:45  | H 0106 | <b>Structural Materials (Steels, light-weight materials, high-temperature materials)</b>                                            |
| MM 70.1–70.5  | Fri | 9:30–11:00  | H 0107 | <b>Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century</b> |
| MM 71.1–71.6  | Fri | 9:30–11:00  | TC 006 | <b>Methods in Computational Materials Modelling (methodological aspect, numerics)</b>                                               |
| MM 72.1–72.4  | Fri | 9:30–10:30  | TC 010 | <b>Magnetic Shape Memory Alloys (joint with MA)</b>                                                                                 |
| MM 73.1–73.9  | Fri | 10:30–12:45 | HL 001 | <b>Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VIII (joint session O/TT/MM/DS/CPP)</b>   |
| MM 74.1–74.4  | Fri | 11:15–12:15 | H 0106 | <b>Structural Materials (Steels, light-weight materials, high-temperature materials)</b>                                            |
| MM 75.1–75.5  | Fri | 11:15–12:45 | H 0107 | <b>Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century</b> |
| MM 76.1–76.5  | Fri | 11:15–12:30 | TC 006 | <b>Methods in Computational Materials Modelling (methodological aspect, numerics)</b>                                               |

## Annual General Meeting of the Metal and Material Physics Division

Wednesday 19:45–20:45 TC 006