



September 22–27, 2024  
Prague Congress Center, Czech Republic

# Errata Sheet

## Talks

### Monday, 23 September

Start	End	Symp.	Location	Title	Speakers	Change	New data
10:00	10:20	C	South Hall 3C	A multiscale CPFE approach for modelling the flow stress response of an austenitic stainless steels under high temperature cyclic loading conditions	Sourabh Supanekar	change of presenter	Speaker: Miguel Espadero
10:40	11:00	C	South Hall 3C	Effect of free surface on the fatigue life of copper	Abhishek Biswas	cancelled	-
13:10	13:30	C	South Hall 3C	Incorporation of temperature dependent coefficients of Voce hardening law in visco-plastic self-consistent model (VPSC) for multiple slip systems implemented in a FEM framework	Johannes Kronsteiner	change of presenter	Speaker: Leo Schwarzmeier
15:30	15:50	C	South Hall 3C	Solute Strengthening predictions based on accurate dislocation core description	Davide Fioravanti	cancelled	-
12:20	12:40	G	North Hall	Computational workflows for experimental materials characterization	Markus Stricker	cancelled	-
13:20	13:40	G	North Hall	Prediction of alloy plasticity fusing textual corpus and physical information: Information density enhancement and knowledge extraction based on MatSciBERT	Zhouran Zhang	new time and date	Tuesday 17:10-17:30
13:30	13:50	H	Chamber Hall	On the origin of interfacial plasticity at twist basal grain boundaries in Ti-Al alloy	Djafar Iabbaden	cancelled	-
14:40	15:10	I	Terrace 2A	Microstructure Classification and the Microstructure State Space	Jeremy Mason	cancelled	-
16:10	16:30	I	Terrace 2A	Limitations of the Classical Driving Forces for Grain Boundary Segregation	Malik Wagih	cancelled	-
18:10	18:30	B	South Hall 3B	Mechanical behaviour of Ni <sub>3</sub> Al free-standing and matrix-embedded metallic nanoparticles at different temperatures: may we explain the tension/compression asymmetry observed in Ni-based superalloys using MD simulations?	Céline Gérard	cancelled	-
17:50	18:10	A	South Hall 2B	Variational Quantum Algorithms for Electronic Structure Calculations	Ivana Miháliková	new time	18:10 – 18:30 same date
18:10	18:30	A	South Hall 2B	Hubbard physics with Rydberg atoms: using a quantum spin simulator to simulate strong fermionic correlations, towards strongly correlated materials modelling	Antoine Michel	new time	18:30 – 18:50 same date
18:30	18:50	A	South Hall 2B	Quantum-computing study of the electronic structure of diamond-structure crystals	Michal Ďuriška	new time	17:50 – 18:10 same date
17:50	18:10	L	Room 221+222	Microstructural Induced Failure Modes in Crystalline Materials	Mohammed Zikry	new time and date	Tuesday 16:00-16:20
18:10	18:30	L	Room 221+222	The Micromechanics of Void Nucleation	Coleman Alleman	new time	17:50 – 18:10 same day

### Tuesday, 24 September

Start	End	Symp.	Location	Title	Speakers	Change	New data
11:50	12:10	G	North Hall	Material Discovery: derivatives of Cantor alloys and complex glasses	Silvia Bonfanti	cancelled	-
14:50	15:00	M	Terrace 2B	Multiscale model of the conductivity of filled diblock copolymer systems	Alexander Chervanyov	cancelled	-
15:30	16:50	K	South Hall 2A	Session Symposium K: Multiscale insights into high and medium entropy alloys: From atomistic calculations to macroscopic applications	Chair: Silvia Bonfanti	change of chair	New chair: Mikko Alava
16:00	16:20	K	South Hall 2A	Critical Assessment of the Interatomic Potential in Cantor alloys: Assessing Metastable Phases and Phase Diagrams of the CoCrFeMnNi system	Stefan Hiemer	cancelled	-
16:00	16:20	L	Room 221+222	An unified fracture model for cleavage and ductile fracture	Junhe Lian	cancelled	Slot used by Mohammed Zikry
17:00	17:20	L	Room 221+222	Fracture behaviour of 4140 steel submitted to annealed, normalized, quench and tempering heat treatments with in-situ hydrogen charging	Afzaal Ahmed	cancelled	-



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## Wednesday, 25 September

Start	End	Symp.	Location	Title	Speakers	Change	New data
9:50	10:20	B	South Hall 3B	Keynote: Microstructural uncertainty: The limits of predictive models for microstructural evolution	Elizabeth Holm	cancelled	-
9:50	10:20	B	South Hall 3B	Keynote: Multiscale Modelling of High Strain Rate Plastic Deformation in Tantalum	Dan Mordehai	new talk	-
9:50	11:40	C	South Hall 3C	Symposium C: Multiscale modeling of crystal plasticity of materials	Vasily Bulatov	change of chair	New chair: Jan Fikar
10:40	11:00	G	North Hall	Machine learning interatomic potentials for carbon-salt thermal energy storage materials	Alexis Front	cancelled	-
12:40	13:10	C	South Hall 3C	Keynote: Predicting metal strength through cross-scale modeling	Nicolas Bertin	cancelled	-
12:40	13:10	O	Chamber Hall	Keynote: Machine learning for next generation additively manufactured structural alloys in extreme environments	S. Mogadeseh Taheri-Mousavi	change of presenter	Speaker: Ben Glaser
13:30	13:50	F	South Hall 3B	Development of Biofidelic Soft Tissues Simulants	Arnab Chanda	cancelled	-
13:50	14:10	F	South Hall 3B	Exploring Gene Regulation through Chromatin Organization: Computational Framework Connecting HiC to Gene Transcription	Hemant Kumar	No show	-
13:50	14:10	F	South Hall 3B	Keynote: Modeling charged polymers for soft materials design	Andrea Giuntoli	added replacement	Replaced Hemant Kumar
15:00	16:50	G	North Hall	Session Symposium G: Machine learning assisted materials discovery	Markus Stricker	change of chair	Thomas Hammerschmidt

## Thursday, 26 September

Start	End	Symp.	Location	Title	Speakers	Change	New data
10:20	10:50	D	Terrace 2B	Keynote: Altermagnetism imaged and controlled down to the nanoscale in MnTe	Peter Wadley	cancelled	-
10:20	10:50	D	Terrace 2B	Keynote: Magnetic Shape Memory Effects in Heusler Alloys- From Macroscopic Description to Nanoscale	Oleg Heczko	new talk	-
10:30	10:50	G	North Hall	Materials Genome Engineering in Steels: Break down the barrier of small sample sizes	Wei Xu	cancelled	-
10:40	11:00	F	South Hall 3B	Computer simulations of membrane models	Andrzej Sikorski	cancelled	-
10:40	11:00	F	South Hall 3B	Discovering dynamic laws from observations: The case of self-propelled, interacting colloids	Chantal Valeriani	added replacement	Replaced Andrzej Sikorski
10:30	10:50	A	South Hall 2B	Diffusion modelling of H isotopes through the W/Cu interface	Yosvany Silva Solís	new talk	originally poster
10:50	11:10	A	South Hall 2B	QM/MM Style Potential Coupling to Accelerate Simulations	Fraser Birks	new talk	originally poster
11:00	11:20	E	South Hall 3A	The machine learning potential for the W-He system to study the nucleation and growth of He bubble	Huiqiu Deng	cancelled	-



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## Posters

### Tuesday, 24 September – Poster session 1

Number	Symp.	Title	Speakers	Change
2	A	QM/MM Style Potential Coupling to Accelerate Simulations	Fraser Birks	<b>changed to talk</b>
6	A	Diffusion modelling of H isotopes through the W/Cu interface	Yosvany Silva Solís	<b>changed to talk</b>
56	A	Ab initio calculations of tensile strength of M <sub>2</sub> CuB (M = Zr, Mo, and W) new possible 211 MAX phases borides.	Ahmed Gueddouh	<b>new poster</b>

### Wednesday, 25 September – Poster session 2

Number	Symp.	Title	Speakers	Change
14	G	Ab initio calculations of tensile strength of M <sub>2</sub> CuB (M = Zr, Mo, and W) new possible 211 MAX phases borides.	Aleksei Egorov	<b>cancelled</b>
34	I	Modeling the growth kinetics and morphology of oxides on chromium-rich steels	Valentin Bellaich	<b>cancelled</b>
64	D	Lutidine catalyzed highly thermal conductive graphite polyimide films via controlling grain size	Xuliang Luo	<b>new poster</b>
65	D	Template free preparation of graphene tubes from polyimide catalyzed by calcium carbonate	Xuliang Luo	<b>new poster</b>
54	M	Simulation of crack propagation in pipe-grade high-density polyethylene	Jan Poduška	<b>cancelled</b>
54	L	Paradox of Reduced Fatigue Life and Oxide Layer Formation from Omitted Low-Amplitude Cycles	Radek Kubiček	<b>new poster</b>
66	M	Propagator-Biased Chain Generation: accurately reverse mapping phase segregated block copolymers	Mateus Garcia Rodolfo	<b>new poster</b>