MULTISCALE MECHANICS, MULTIPHYSICS MODELING AND SIMULATIONS FOR ENERGY STORAGE

29 August – 31 August 2022, Sirmione, Lake of Garda, Italy

Under the aegis from:

Sponsors

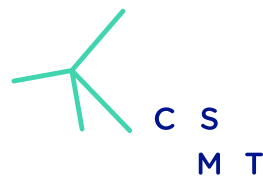| Monday Aug. 29		
Session 1	*Opening – Chairman A. Salvadori*	
8:30	8:50	Lavelli, L. – Major of the Municipality of Sirmione
		Tira, M. – Rector of the University of Brescia
		Zorzella, E. – President of CSMT
		Gaboardi, S. – President of the Mobility Cluster RL
8:50	9:10	Mastinu, G. – Politecnico di Milano - "The automotive cluster of Lombardy: an excellent network from Europe"
9:10	9:30	Perego, O. – RSE – "Lombardy Energy Cleantech Cluster support to the innovation and competitiveness of regional battery sector"

Monday Aug. 29		
Session 1	*Social and industrial challenges.* *Chairman G. Mastinu, Politecnico di Milano*	
9:45	10:15	Knobbe, E. – BMW - "Challenges to simulate interaction of mechanics and electro-chemistry in battery cells – perspective of a cell developer."
10:15	10:45	Oancea, V. – Dassault Systemes - "Challenges to simulate interaction of mechanics and electro-chemistry in battery cells – perspective of a software developer."
		Q&A
		Coffee break
Session 2	*Manufacturing, designing, and processing of battery cells.* *Chairman E. Knobbe*	
11:15	11:45	Pannala, S. – Sabic - "How multiscale modeling of Lithium Ion Batteries for Safety and Performance helped to redesign a cell to achieve dense and safe battery packs?"
11:45	12:15	Franco, A. – Université de Picardie Jules Verne - "Digitalization of Battery Manufacturing using Multiscale Modeling and Machine Learning"
12:15	12:45	Kwade, A. – TU Braunschweig - "Modelling processing and resulting mechanical and transport properties of lithium ion battery electrodes using DEM"
		Lunch break

Session 3	*Imaging and image-based modeling* *Chairman A. Franco*	
14:15	14:45	Figgemeier, E. – RWTH Aachen - "Mechanical Aspects of Ageing in Lithium-Ion Batteries Probed by Computer Tomography and Optical Means"
14:45	15:15	Shearing, P. – UCL - "Multi-scale imaging and modelling of coupled phenomena in battery materials and devices"
15:15	15:45	Schmidt, V. – Universität Ulm - "Stochastic microstructure modeling of battery electrode materials based on 3D image data - a prerequisite for virtual materials testing"
		Coffee break
Session 4	*Interface mechanisms* *Chairman V. Deshpande*	
16:15	16:45	Qi, Y. – Brown University - "When electrons meet ions, multiscale modeling of interfaces in Li-ion Batteries"
16:45	17:15	Guo, K. – A*STAR Singapore - "Interfacial Degradation Mechanisms in Thin Film Electrodes"
17:15	17:45	Vegge, T. – Technical University of Denmark - "ML-accelerated simulations of solid-electrolyte interfaces in electrochemical systems"
17:45	18:15	Wall, W. – Technical University of Munich - "Electro-chemo-thermo-mechanical modeling of all solid-state batteries with a focus on interfaces, uncertainties and inverse analysis"

Tuesday Aug. 30		
Session 5	*Experimental investigations with solid and multicomponent electrolytes.* *Chairman U. Krewer*	
9:00	9:30	Sheldon, B. – Brown University - "Chemo-mechanical phenomena in solid electrolytes"
9:30	10:00	Canepa, P. – NUSingapore - "Millisecond Ion-Transport in Solid Electrolytes"
10:00	10:30	Monroe, C. – University of Oxford - "Ion transport and mechanics in multicomponent battery electrolytes"
		Coffee break
Session 6	*ASSB processes and models* *Chairman A. Latz*	
11:00	11:30	Krewer, U. – Karlsruhe Institute of Technology - "Model-based insight into Li-ion batteries – from cradle to grave"
11:30	12:00	Siegel, D. – UT Austin - "Chemo-mechanical phenomena of relevance for solid state batteries: an atomic scale perspective"
12:00	12:30	Mc Dowell, M. – GeorgiaTech - "Operando Experiments for Understanding the Chemo-Mechanics of Solid-State Batteries"
		Lunch break
Session 7	*Modeling Damage and Failure in ASSB – I* *Chairman G. Bucci*	
14:00	14:30	Deshpande, V. – University of Cambridge - "Failure mechanisms in solid electrolyte Li-ion cells: from void growth in anodes to cracking of electrolytes"
14:30	15:00	Xu, B. – TU Darmstadt - "Chemo-mechanical damage modeling and simulation of solid-state Li-ion battery materials"
15:00	15:30	McMeeking, R. – University of California, Santa Barbara - "Models for storage particle delamination and electrolyte cracking in cathodes of solid state batteries."
15:30	16:00	Ciucci, F. – HKUST, Hong Kong - "Modeling the Defect Chemistry, Transport Properties, and Stability of Anti-perovskite Materials."
19:30		Poster session and social dinner Winery Borgo la Caccia, Pozzolengo

Wednesday Aug. 31		
Session 8	*Modeling Damage and Failure in ASSB – II* *Chairman M. Kamlah*	
9:00	9:30	Martinez-Paneda, E. – Imperial College - "A phase field electro-chemo-mechanical model for predicting void evolution at the Li-electrolyte interface in all-solid-state batteries"
9:30	10:00	Bucci, G. – Palo Alto Research Center - "Chemo-mechanics and microstructural design of solid-state batteries"
10:00	10:30	Di Leo, C. – GeorgiaTech - "Continuum gradient theories for diffusion-reaction-deformation in solids: Application to conversion electrodes and Li filament growth."
		Coffee break
Session 9	*Modeling and simulations – I* *Chairman W. Wall*	
11:00	11:30	Smith, K. – NREL - "Frontiers in Simulation of Battery Chemo-Mechanical Physics and Degradation"
11:30	12:00	Kamlah, M. – Karlsruhe Institute of Technology - "Interaction of diffusion and transport with mechanics in active materials and electrodes for electrochemical energy storage"
12:00	12:30	Latz, A. – Universität Ulm - "Impact of structure and chemo – mechanical coupling on degradation in Lithium-Ion batteries"
		Lunch break
Session 10	*Modeling and simulations – II* *Chairman E. Martinez-Paneda*	
14:00	14:30	Danilov, D. – Technical University of Eindhoven - "Mathematical modeling as an approach to the investigation of electrochemical storage"
14:30	15:00	Salvadori, A. – University of Brescia - "Recent advances in modeling and simulations of gel polymer and ceramic electrolytes"
15:00	15:30	Runesson, K. – Chalmers University of Technology - "Aspects on the computational modeling of structural batteries"
	Closure – E. Knobbe, R. McMeeking	