

# Workshop on Digitalization and Automation Boost Energy Materials Research

**24-25 January 2024 – CNR Headquarter  
Piazzale Aldo Moro, 7 - 00185 Rome, Italy**

## Programme Day 1

8:15	<b>Registration</b>
8:30	<b>Welcome</b> by COST-Action Chair, Workshop Organizer, CNR Director
8:45	<b>EU-MACE Management committee meeting</b>
11:00	<b>WS attendees arrival and registration</b>
11:30	<b>Workshop opening</b> by EU-MACE/EERA – JP AMPEA & DfE
11:40	<b>Invited speaker: Natalia Konchakova (HEREON)</b> VIPCOAT and IM4EU/ Open Innovation Platform (to be confirmed)
12:20	<b>Refreshment &amp; Poster session</b>
14:00	<b>Hernán Asorey (CIEMAT, Spain)</b> A digital framework for adoption FAIR principles and its implementation in the solar radiation field
14:20	<b>August Wierling (Western Norway University of Applied Sciences, Norway)</b> Demonstrating how energy data can comply with FAIR data principles avoiding large efforts and specialized skills by using csv on the web
14:40	<b>Kourosh Malek (FZ-Jülich, Germany)</b> Novel approaches in meta-data management and ontologies for clean energy materials
15:00	<b>Josua Vieten (ExoMatter, Germany)</b> "Fast and efficient screening of materials for thermochemical energy storage on a novel materials informatics platform"
15:20	<b>Massimo Celino (ENEA, Italy)</b> IEMAP: Italian Energy Materials Acceleration Platform
15:40	<b>Coffee break</b>
16:00	<b>JP-AMPEA Steering Committee meeting</b>
18:15	<b>End of Day 1</b>

Dinner information: to be announced on Day 1

## Programme Day 2

08:30	<b>Arrival &amp; Registration</b>
09:00	<b>Anja Bieberle-Hütter (DIFFER, the Netherlands)</b> Multiscale modeling of electrochemical interfaces: Challenges and chances
09:20	<b>Viktor Mandrolko (Univ. Lorraine, France)</b> Understanding heat transport across functionalized silica water interface: insights from molecular dynamics simulations
09:40	<b>Nima E. Gorji (TU Dublin, Ireland)</b> Multi-physics COMSOL Simulation of Five Heat Generation Factors
10:00	<b>Ainhoa Bustinza (CIC energiGUNE, Spain)</b> Development of automated high-throughput modules for accelerated discovery of new battery materials
10:20	<b>Theodoros Dimopoulos (AIT, Austria)</b> Solar cell performance characterization through combinatorial deposition and automatized I-V measurements and analysis
10:40	<b>Short break</b>
11:00	<b>Invited speaker: Anjuli Szawiola (NRCan, Canada)</b> Training & knowledge dissemination: a case study in building international networks
11:40	<b>Refreshment &amp; Poster session</b>
13:30	<b>Supriya Nandy (VTT, Finland)</b> Automated defect detection workflow using SEM and ML algorithm: development towards self-driven materials design and innovation
13:50	<b>Selçuk Yerci (METU, Turkey)</b> Bayesian optimization with experience for fast development of monolithic tandem solar cells: simulation case stud
14:10:00	<b>Michael Eikerling (FZ-Jülich, Germany)</b> Accelerating the design and integration of electrocatalyst materials for hydrogen technologies with theory and computation
14:30:00	<b>Mauro Palumbo (UniTo, Italy)</b> ML assisted development of metallic hydrides
14:50:00	<b>Filippos Sofos (UTH, Greece)</b> Materials properties extraction with interpretable artificial intelligence
15:10:00	<b>Coffee break</b>
15:30:00	<b>Round-Table discussion</b>
17:00:00	<b>Conclusion &amp; closing</b>
17:15:00	<b>Convivial networking</b>
18:00:00	<b>End</b>

## List of Posters

<b>Oleg Olikh (KNU, Ukraine)</b> Characterization of impurity contamination in solar cells with the assistance of machine learning
<b>Pablo Alvarez (Uni Oviedo, Spain)</b> Advanced materials for hydrogen liquefaction and transportation
<b>Leonarda Liotta (ENEA, Italy)</b> Toward the IEMAP: database implementation with perovskite oxide materials for electrolyzers
<b>Lesia Chepela (KNU, Ukraine)</b> Thermal conductivity study of nanocomposite systems made of porous silicon and liquids
<b>José A. Moriñigo (CIEMAT, Spain)</b> Novel ideas in preconditioning iterative solvers for PDEs solving
<b>Ali Ercetin (Bandirma U, Turkey)</b> Integrating experimental and computational techniques for enhanced characterization of material properties: A focus on dislocation densities and residual stresses
<b>Martina Palermo (UniRoma, Italy)</b> An equivalent circuit model based analysis for the energy conversion chain from PV source with supercapacitor as DC-link
<b>Carlos Nieto-Draghi (IFP Energies Nouvelles, France)</b> A New Class of Descriptors for Nanoporous Materials and its Applications to Classification and CO <sub>2</sub> Gas Adsorption in Zeolites