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	**Registration**
8:30	**Welcome** by COST-Action Chair, Workshop Organizer, DIITET CNR Director
8:45	**EU-MACE Management committee meeting**
11:00	**WS attendees arrival and registration**
11:30	**Workshop opening** by EU-MACE/EERA – JP AMPEA & DfE
11:40	**Invited speaker: Natalia Konchakova (Helmholtz-Zentrum Hereon, Germany)** VIPCOAT Supporting the European Green and Digital Transition by Digitalizing Innovative Advanced Materials: VIPCOAT, DigiPass and IAM4EU
12:20	**Refreshment & Poster session**
14:00	**Hernán Asorey (CIEMAT, Spain)** A digital framework for adoption FAIR principles and its implementation in the solar radiation field
14:20	**August Wierling (Western Norway University of Applied Sciences, Norway)** Demonstrating how energy data can comply with FAIR data principles avoiding large efforts and specialized skills by using csv on the web
14:40	**Kourosh Malek (FZ-Jülich, Germany)** Novel approaches in meta-data management and ontologies for clean energy materials
15:00	**Josua Vieten (ExoMatter, Germany)** "Fast and efficient screening of materials for thermochemical energy storage on a novel materials informatics platform"
15:20	**Massimo Celino (ENEA, Italy)** IEMAP: Italian Energy Materials Acceleration Platform
15:40	**Coffee break**
16:00	**JP-AMPEA Steering Committee meeting**
18:15	**End of Day 1**

Dinner information: to be announced on Day 1

Programme Day 2

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

17:00:00	**Conclusion & closing**
17:15:00	**Convivial networking**
18:00:00	**End**

List of Posters

Oleg Olikh (KNU, Ukraine) Characterization of impurity contamination in solar cells with the assistance of machine learning
Pablo Alvarez (Uni Oviedo, Spain) Advanced materials for hydrogen liquefaction and transportation
Leonarda Liotta (CNR, Italy) Toward the IEMAP: database implementation with perovskite oxide materials for electrolyzers
Lesia Chepela (KNU, Ukraine) Thermal conductivity study of nanocomposite systems made of porous silicon and liquids
José A. Moriñigo (CIEMAT, Spain) Novel ideas in preconditioning iterative solvers for PDEs solving
Ali Ercetin (Bandirma U, Turkey) Integrating experimental and computational techniques for enhanced characterization of material properties: A focus on dislocation densities and residual stresses
Martina Palermo (UniRoma, Italy) An equivalent circuit model based analysis for the energy conversion chain from PV source with supercapacitor as DC-link
Carlos Nieto-Draghi (IFP Energies Nouvelles, France) A New Class of Descriptors for Nanoporous Materials and its Applications to Classification and CO2 Gas Adsorption int Zeolites