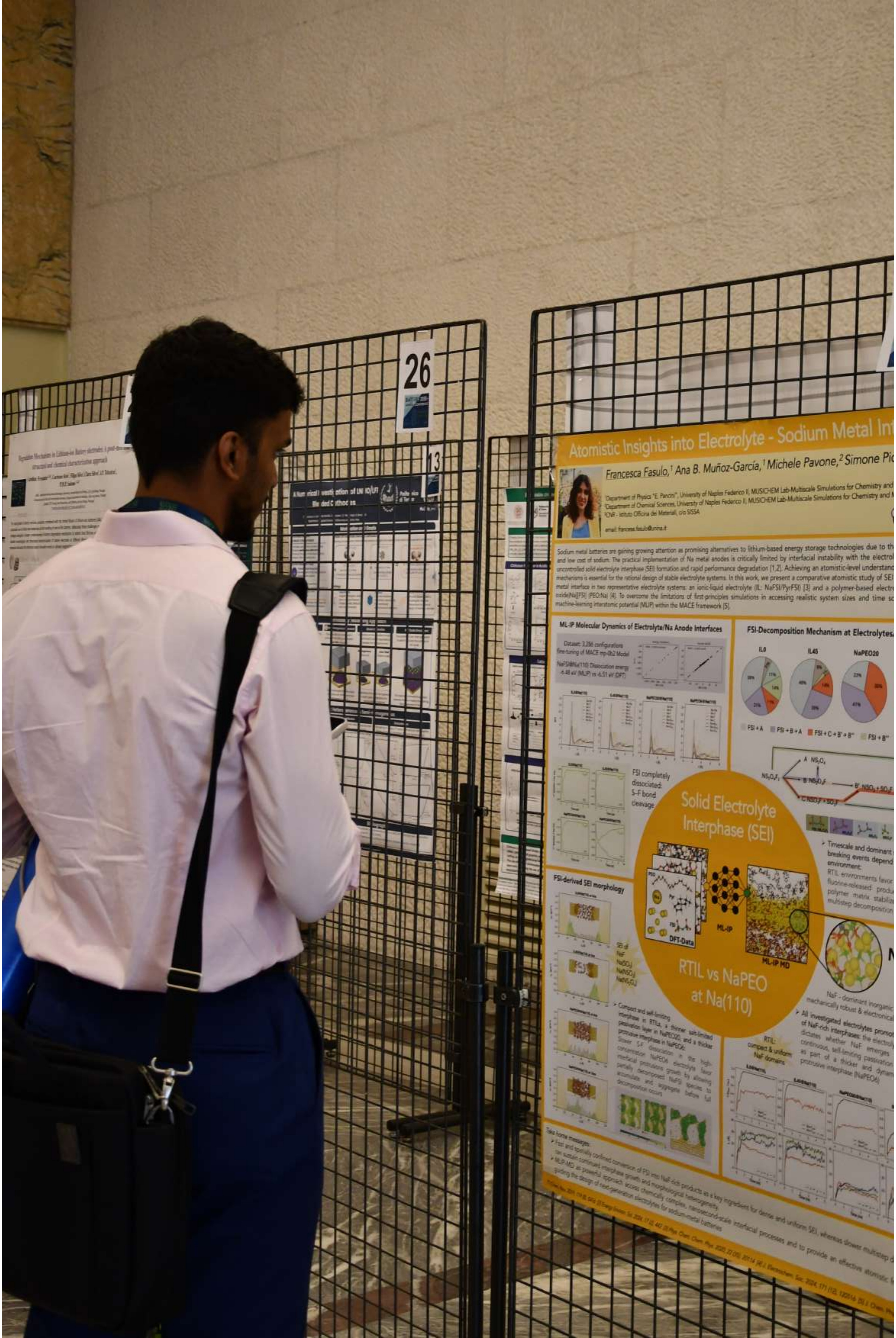
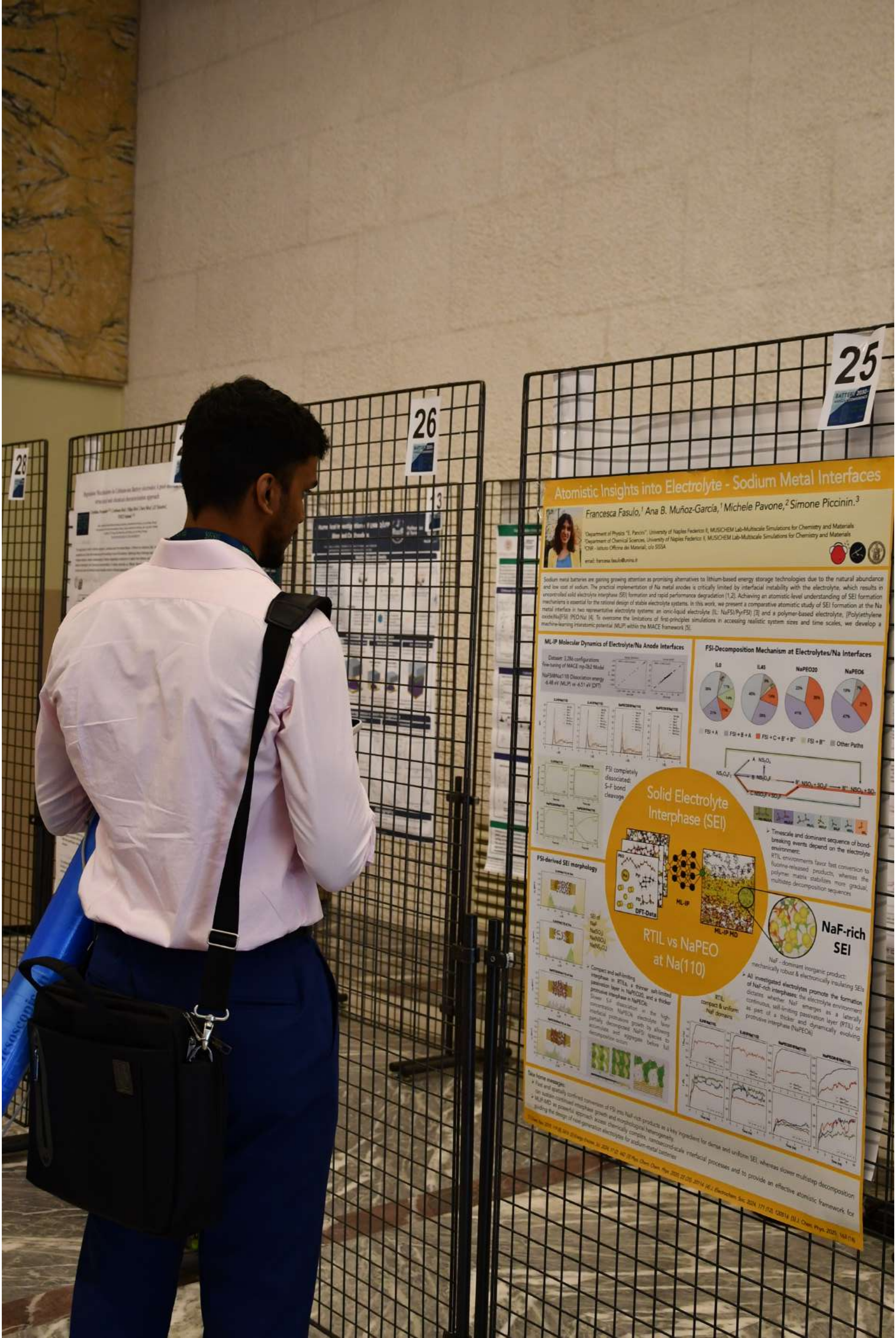

DAY 2
BATTERY 20
ANNUAL CONFE
7-8 M
Turi
BATTERY 2030+


BATTE
ANNUAL


BATTER
ANNUAL


26
13
Atomistic Insights into Electrolyte - Sodium Metal In
Francesca Fasulo,1 Ana B. Muñoz-García,1 Michele Pavone,2 Simone Pi
ML-IP Molecular Dynamics of Electrolyte/Na Anode Interfaces
FSI-Decomposition Mechanism at Electrolytes
Solid Electrolyte Interphase (SEI)
RTIL vs NaPEO at Na(110)
FSI-derived SEI morphology
ML-IP
DFT-Data
ML-IP MD



Atomistic Insights into Electrolyte - Sodium Metal Interfaces

Francesca Fasulo,[1] Ana B. Muñoz-García,[1] Michele Pavone,[2] Simone Piccinin.[3]

[1]Department of Physics "E. Pancini", University of Naples Federico II, MUSICHEM Lab-Multiscale Simulations for Chemistry and Materials
[2]Department of Chemical Sciences, University of Naples Federico II, MUSICHEM Lab-Multiscale Simulations for Chemistry and Materials
[3]CNR - Istituto Officina dei Materiali, c/o SISSA

email: francesca.fasulo@unina.it

Sodium metal batteries are gaining growing attention as promising alternatives to lithium-based energy storage technologies due to the natural abundance and low cost of sodium. The practical implementation of Na metal anodes is critically limited by interfacial instability with the electrolyte, which results in uncontrolled solid electrolyte interphase (SEI) formation and rapid performance degradation (1,2). Achieving an atomistic-level understanding of SEI formation mechanisms is essential for the rational design of stable electrolyte systems. In this work, we present a comparative atomistic study of SEI formation at the Na metal interface in two representative electrolyte systems: an ionic-liquid electrolyte (IL: NaFSI/PyrFSI) [3] and a polymer-based electrolyte, [Poly(ethylene oxide)Na(FSI) (PEO:Na) [4]. To overcome the limitations of first-principles simulations in accessing realistic system sizes and time scales, we develop a machine-learning interatomic potential (MLIP) within the MACE framework [5].

ML-IP Molecular Dynamics of Electrolyte/Na Anode Interfaces

Dataset: 3,286 configurations
Fine-tuning of MACE mp-0b2 Model

NaFSI@Na(110) Dissociation energy
-6.48 eV (MLIP) vs -6.51 eV (DFT)

FSI completely dissociated: S–F bond cleavage

FSI-Decomposition Mechanism at Electrolytes/Na Interfaces

- Timescale and dominant sequence of bond-breaking events depend on the electrolyte environment:

RTIL environments favor fast conversion to fluorine-released products, whereas the polymer matrix stabilises more gradual, multistep decomposition sequences

Solid Electrolyte Interphase (SEI)

RTIL vs NaPEO at Na(110)

FSI-derived SEI morphology

SEI of NaF Na_2SO_3 $NaNSO_2$ $NaNS_2O_3$

- Compact and self-limiting interphase in RTILs, a thinner self-limited passivation layer in NaPEO20, and a thicker protrusive interphase in NaPEO6.

Slower S–F dissociation in the high-concentration NaPEO6 electrolyte favor interfacial protrusions growth by allowing partially decomposed NaFSI species to accumulate and aggregate before full decomposition occurs.

NaF-rich SEI

NaF - dominant inorganic product: mechanically robust & electronically insulating SEIs

- **All investigated electrolytes promote the formation of NaF-rich interphases:** the electrolyte environment dictates whether NaF emerges as a laterally continuous, self-limiting passivation layer (RTIL) or as part of a thicker and dynamically evolving protrusive interphase (NaPEO6)

RTIL compact & uniform NaF domains

Take home messages:

- Fast and spatially confined conversion of FSI into NaF-rich products as a key ingredient for dense and uniform SEI, whereas slower multistep decomposition can sustain continued interphase growth and morphological heterogeneity.
- MLIP-MD as powerful approach to access chemically complex, nanosecond-scale interfacial processes and to provide an effective atomistic framework for guiding the design of next-generation electrolytes for sodium-metal batteries


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
BATTERY
2030+
ATTERY 2030+
NNUAL CONFERENCE
7-8 May 2026
Turin, Italy


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico di Torino
1859


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico
di Torino
1859


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico di Torino
1859


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico di Torino
1859
ATTERY 2030+
TTERY 2030+
UAL CONFERENCE
-8 May 2026
Turin, Italy


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico di Torino
1859


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico
di Torino


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico
di Torino
1859


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico di Torino


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico
di Torino
1859
BATTERY 2030+
ANNUAL CONFERENCE


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico
di Torino
1859
BATTERY 2030+
ANNUAL CONFERENCE


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico di Torino
BATTERY 2030+


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico di Torino


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico
di Torino
1859
BATTERY 2030+
ANNUAL CONFERENCE


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico di Torino
BATTERY 2030+
ANNUAL CONFERENCE
Turin, Italy


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico
di Torino
1859


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico di Torino
1859


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico di Torino


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico di Torino
1859


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico
di Torino
1859


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico
di Torino
1859


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico di Torino


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico di Torino


DAY 2
BATTERY 2030+
ANNUAL CONFERENCE
Politecnico


DAY 2
BATTERY 203
ANNUAL CONFERE
7-8 May
Turin,
BATTERY 2030+
BATTERY 2030
AT THE HEART OF A CONNECTED GREEN SOCIETY
WWW.BATTERY2030.EU


DAY 2
BATTERY 203
ANNUAL CONFEREN
7-8 May 2
Turin,
BATTERY 2030+
BATTERY 2030
AT THE HEART OF A CONNECTED GREEN SOCIETY
WWW.BATTERY2030.EU


DAY 2
BATTERY 20
ANNUAL CONFER
7-8 Ma
Turin,
BATTERY 2030+


DAY 2
BATTERY 20
ANNUAL CONFER
7-8 Ma
Turin
BATTERY 2030+


DAY 2
BATTERY 20
ANNUAL CONFE
-8 M
Turi
BATTERY 2030+