ENERGETICS

INRiM - Construction and metrological validation of digital models (digital twins) for materials and energy storage devices

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Context of the research activity	Development of digital twins for describing transport and reactive phenomena within materials for energy storage in electrochemical batteries
Objectives	The main research activity will focus on the development of digital twins for describing transport and reactive phenomena within materials for energy storage in electrochemical batteries (e.g., Li-ion batteries), with the final aim to deepening our current understanding on the irreversible phenomena occurring within electro-chemical cells leading to degradation processes and capacity fade. The project is funded by the Italian Ministry of Research and will be carried out at Politecnico di Torino (i.e. Multi-Scale Modeling Laboratory – SMaLL: www.polito.it/small), at the Italian Metrological Institute – INRIM (https://www.inrim.it/en) and in collaboration with other leading research groups both in Italy and Europe. Main responsibilities and duties are listed below: • Develop and implement state-of-the-art atomistic models including machine learning and neural network potential based algorithms to study electrochemical battery materials; • Build digital twin models to describe transport and reactive phenomena within materials for energy storage in electrochemical batteries; • Utilize data from atomistic simulations (reactive molecular dynamics based on machine learning ML force fields, classical molecular dynamics, mesoscopic models such as kMC), experimental data extracted from literature, and generated through accurate metrological characterization (e.g., through Atomic Force Microscopy or Transmission Electron Microscopy); • Use computational tools based on molecular dynamics and artificial intelligence algorithms to produce accurate and multiscale atomistic models of electrode-electrolyte interfaces; • Analyze and interpret simulation results to gain insights into the

	mechanisms governing battery performance; • Collaborate with experimental researchers to validate simulation results and guide the design of new battery materials.

Skills and competencies for the development of the activity	Basic knowledge on applied thermodynamics. Basic knowledge on computational modelling and programming