POLITECNICO DI MILANO

PhD in INGEGNERIA DEI MATERIALI / MATERIALS ENGINEERING - 38th cycle

PNRR_352 Research Field: PHYSICO-CHEMICAL MODEL OF LITHIUM BATTERIES INCLUDING REDOX REACTIONS, TRANSPORT PHENOMENA (ELECTRODES AND ELECTROLYTE) AND DEGRADATION PHENOMENA

Monthly net income of PhDscholarship (max 36 months)
€ 1400.0 In case of a change of the welfare rates during the three-year period, the amount could be modified.

Context of the research activity	
Motivation and objectives of the research in this field	Lithium-ion and lithium-metal batteries are expected to play a key role in exploitation of renewable energy sources, as well as more environmentally friendly electric mobility. In turn, sustainable energy and mobility are core elements for the "green transition", in Italy's national plan for recovery and resilience (PNRR). These batteries are complex assemblies, with a time-dependent nano- and micro-structure.[1] Irreversible degradation processes may take place during charge and discharge cycles, compromising their function, first in a gradual way and then catastrophically. These degradation processes differ in detail, but they are typically of a chemo-mechanical nature. Considering for example charging processes, the solid phases where the lithium ions deposit or intercalate (metallic lithium films, or graphite or silicon nanoparticles, for example) may undergo substantial volume changes, possibly is a strongly anisotropic and irregular fashion. This generates mechanical stresses, that may produce in turn microcracks, perforation of the solid-electrolyte interface by dendrites, changes in morphology, losses of active material, and battery short circuits.The aim of the research will be to develop, validate and apply methods to simulate lithium-based batteries on a computer, in order to improve our understanding of their chemo-mechanical behavior and use this information to optimize their performance, safety and durability. The computational

	methods developed for these systems may be extended and applied also to other types of electrochemical storage devices. [1] Sun, Y.; Liu, N.; Cui, Y. Promises and Challenges of Nanomaterials for Lithium-Based Rechargeable Batteries. *Nat. Energy* **2016**, *1* (7), 16071.
Methods and techniques that will be developed and used to carry out the research	The batteries will be modelled with a particle-based coarse-grained model, originally developed by Dr. Enrico Masoero (Cardiff University, UK) to study chemo-mechanical phenomena in construction materials. Charge and discharge processes are represented by the formation and dissolution of solid particles at the electrodes. In a kinetic Monte Carlo approach, the rates of these processes depend on the local concentration of the ions within the electrolyte and on the currents (or the potentials) imposed at the electrodes. The effective interaction between the particles making up each solid phase may be chosen so as to reproduce their respective mechanical properties (e.g., shear and bulk elastic moduli). This type of approach allows a consistent description of both chemical and mechanical processes, and therefore also of their coupling. The research will be carried out in close collaboration with ENI SpA, where these materials and processes are investigated experimentally. The research will thus benefit from and support ENI's research efforts, in the transition from a hydrocarbon-based economy to one based on clean, renewable energies. The increased synergy between industry and academia, between fundamental and applied research, are perfectly consistent with Italy's PNRR. [2] Shvab, I.; Brochard, L.; Manzano, H.; Masoero, E. Precipitation Mechanisms of Mesoporous Nanoparticle Aggregates: Off-Lattice, Coarse-Grained, Kinetic Simulations. *Cryst. Growth Des.* **2017**, *17* (3), 1316¿1327.
Educational objectives	• Educate the candidates to critical, rational thinking. • Foster an attitude to continuing education and self-improvement. • Learn to communicate effectively, both in writing and orally.

	• More technical skills: properties ot materials, scientific computing.
Job opportunities	Research in renewable energies, new materials, numerical simulation of complex systems, statistical data analysis, teaching and higher education. Development of new materials and optimization of their production processes in high-tech companies, requiring quantitative reasoning and good communication skills.
Composition of the research group	2 Full Professors 3 Associated Professors 1 Assistant Professors 4 PhD Students
Name of the research directors	Prof. Guido Raos

Contacts
email: guido.raos@polimi.itgroup web site: https://3most.chem.polimi.it/

Additional support - Financial aid per PhD student per year (gross amount)	
Housing - Foreign Students	--
Housing - Out-of-town residents (more than 80Km out of Milano)	--

Scholarship Increase for a period abroad	
Amount monthly	700.0 €
By number of months	6

National Operational Program for Research and Innovation	
Company where the candidate will attend the stage (name and brief description)	Eni SpA
By number of months at the company	6
Institution or company where the candidate will spend the period abroad (name and brief description)	TBD
By number of months abroad	6

Additional information: educational activity, teaching assistantship, computer availability, desk availability, any other information
Confidentiality: since this is a thematic scholarship, the management of Confidential Information, Results and their publication is subordinate to the restrictions agreed upon with the funding company. Upon acceptance of the scholarship, the beneficiary must sign a specific commitment.

Individual budget for research (during the 3 years): about 5.400 euro

Teaching assistantship: availability of funding in recognition of supporting teaching activities by the PhD student.There are various forms of financial of for activities of support to the teaching practice. The PhD student is encouraged to take part in these activities within the limits allowed by the regulation.