Dipartimento di Chimica – Università di Torino

Proposte di TESI: Gruppo Materiali Metallici

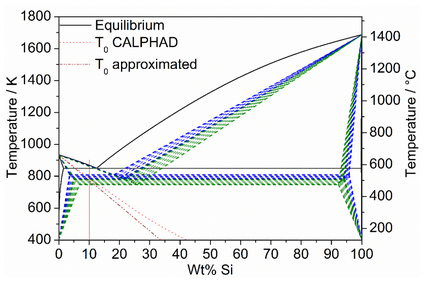
Additive manufacturing

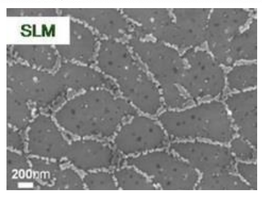
DESCRIPTION: 3D printing is a new production method that allows a highly customized production, minimizing stock and components weight reduction

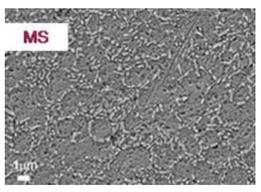
OBJECTIVES: Studies on the influence of process conditions:

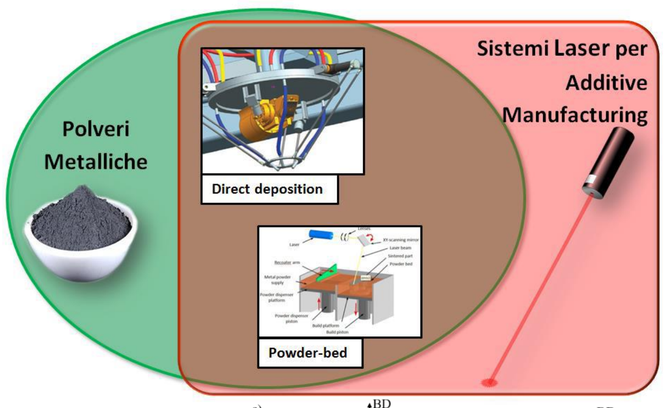
1) Phase selection (non-equilibrium phase diagram calculations)
2) Microstructures
3) Mechanical properties

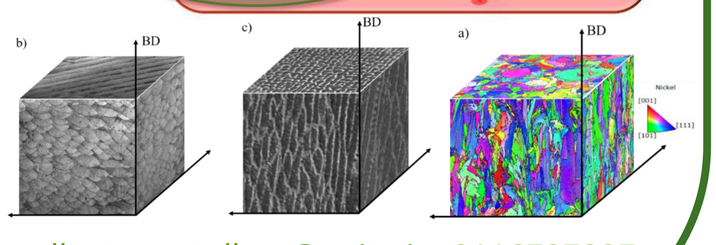
APPROACHES: Simulation of additive manufacturing processes by rapid solidification of alloys. Synthesis of alloys, characterisation by XRD, SEM, TEM, EDS, EBSD, DSC, mechanical properties.











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Advanced sensors and antibacterial surfaces

DESCRIPTION: Nanoporous metals are a new class of materials characterised by a high surface area and advanced optical and catalytic properties. The design of the size and morphology of ligaments and pores, by which the material is constituted, enables to access peculiar properties for biosensors, catalysis, antibacterial applications

OBJECTIVES:

1) Design of Au nanoporous metals starting from metastable precursors (Au-Fe, Au amorphous alloys)
2) Study of mechanism and kinetics of de-alloying, ligament morphology formation
3) Design of Ti/TiO_2 nanoporous metals for antibacterial applications Microstructures

APPROACHES: Alloy synthesis, dealloying techniques (free corrosion, electrochemical dealloying), structural and microstructural characterisation (SEM, TEM, EDS, XRD, EBSD), calorimetry, electrochemistry, SERS, Raman. Work done in collaboration with PhD students.

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Solidification of industrial alloys

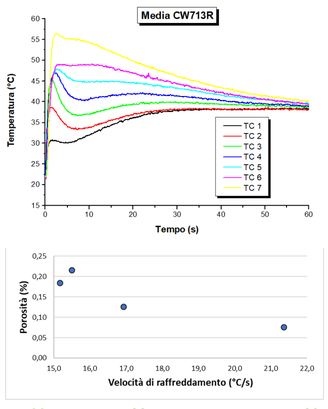
DESCRIPTION: collaboration with industrial partners aimed to optimize the solidification processes of finished components or semi-finished shapes.

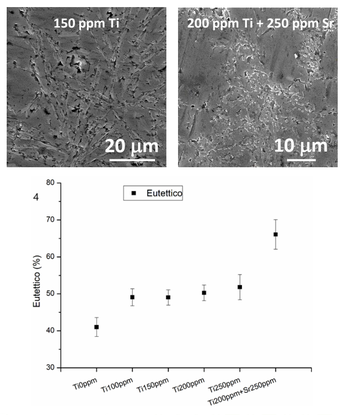
OBJECTIVES:

1) Reduction of defects and waste in industrial processes
2) Improvement of process and material sustainability within the ″circular economy″ paradigm

APPROACHES:

1) Use of lab scale apparatus (TopCast) to evaluate the effects of process parameters (cooling rate) on the defects formation and microstructure in the as cast state
2) Use of modifiers to tailor microstructure and mechanical properties in the as cast state with the aim to eliminate or reduce the impact of thermal treatments (e.g. Al-alloys)
3) Use of secondary recycled Al alloys and comparison of their properties with respect to primary alloys





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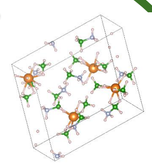
Modelling of metallic materials and materials for energy

ICSC Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

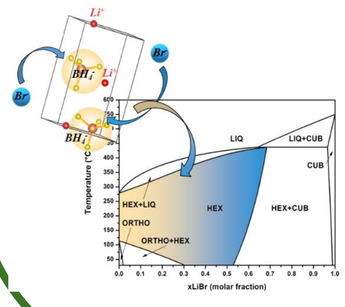


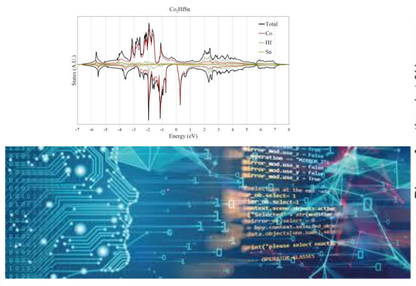
DESCRIPTION: material modelling has become an essential tool for understanding and predicting material characteristics and properties, and for the development of new materials and processes in a shorter time and at a lower cost. From a "multiscale" perspective, modelling can take place starting from fundamental models on atomic scales and then scaling up to macroscopic systems and properties.

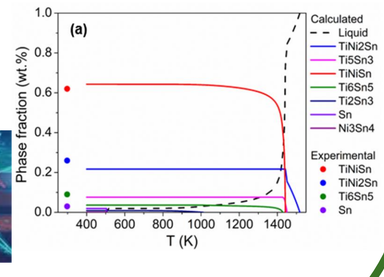
OBJECTIVES:

1) Quantum mechanics methods based on Density Functional Theory (DFT) for the determination of materials properties
2) Simulation of phase transformations
3) Development of thermodynamic databases and calculation of phase diagrams by CALPHAD method
4) Development and applications of machine learning models for materials

APPROACHES: Plane-Wave DFT (VASP, Quantum Espresso), CALPHAD method with ThermoCalc and Pandat software, machine learning with Python, Scikit-Learn and Tensorflow.







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Proposte di TESI: Gruppo Materiali Metallici

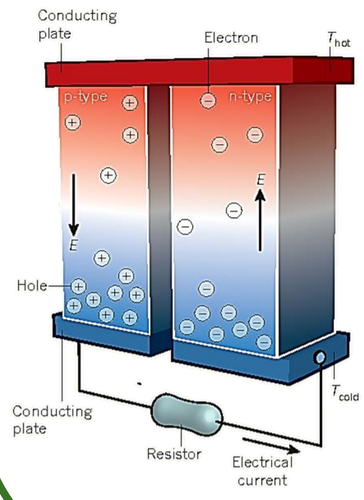
Thermoelectric materials for waste heat harvesting

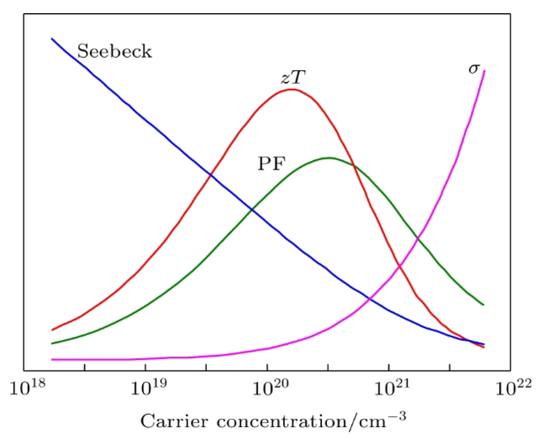
DESCRIPTION: Waste heat from industrial processes, automotive exhaust, domestic appliances can be converted to electricity through Seebeck effect. Thermoelectric generators (TEGs) are based on semiconductors with optimized figure of merit ZT.

OBJECTIVES:

1) Doping control for adjusting carrier concentration and optimizing power factor ($\alpha^2\sigma$)
2) Microstructure refinement to decouple electronic (κ_{el}) and lattice thermal conductivity (κ_{ph})

APPROACHES: Use of non equilibrium metallurgical processing routes (rapid solidification and mechanical alloying) to favour microstructural refinement. Correlation between process, structure, microstructure and properties.





$$\uparrow ZT = \frac{\alpha^2 \sigma T}{\kappa_{el} + \kappa_{ph}} \downarrow$$

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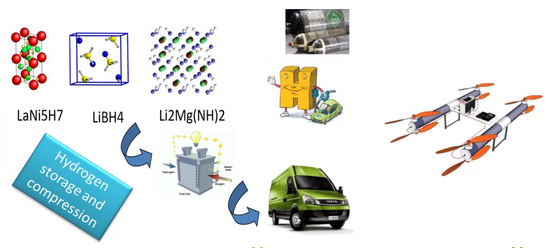
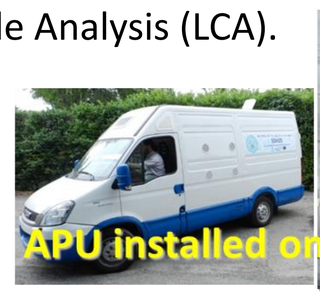
Hydrogen storage, compression and purification for energy systems

DESCRIPTION: Need to optimize and develop materials for the storage, compression and purification of H_2 in renewable energy and biomass pyrolysis systems. Projects: HyCARE H2020 (https://hycare-project.eu); UNITA GFI; EX-MACHINA; CN PNNR MOST; Fuel Cells and Hydrogen Joint Undertaking; Regione Piemonte.

OBJECTIVES: Development of new materials and processes to optimize the storage and compression of H_2 as an energy carrier for stationary and mobile applications. Solid state hydrogen storage from renewable sources. Integration with hydrogen fuel cells. Recovery and purification of H_2 in contaminated streams from biomass treatments. Definition of materials' properties by experiments and Machine Learning.

APPROACHES: Development of advanced materials: complex hydrides and intermetallics with suitable hydrogenation properties. Study of: phase transformation; phase diagram calculations (CALPHAD); Life Cycle Analysis (LCA).





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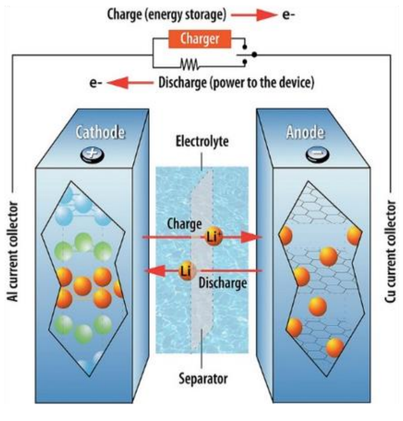
Materials for Li-ion and solid-state batteries

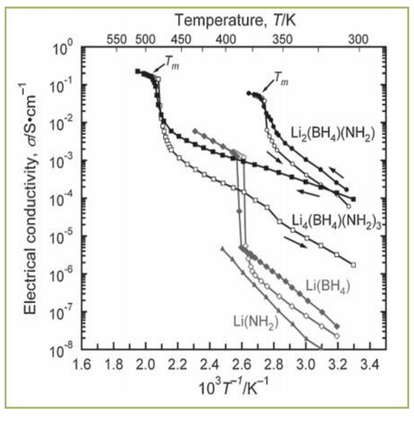
DESCRIPTION: Development of improved materials for electrodes and solid-state electrolytes for batteries to foster energy storage from renewable energies.

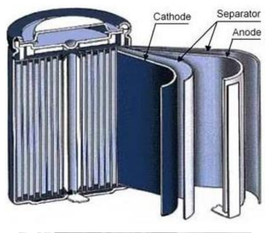
OBJECTIVES:

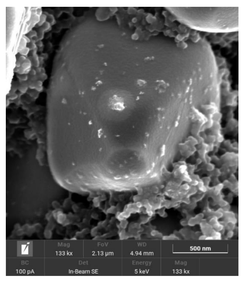
1) Production and testing of innovative anodic and cathodic materials for batteries
2) Li^+ and Mg^{2+} high-conductive materials as solid-state electrolytes

APPROACHES: Materials synthesis by ball milling. Structural and thermal characterization by XRD and DSC. Electrochemical characterization by incremental capacity analysis. Battery performance testing by EIS and thermal/electric cycles. Density functional theory simulation of diffusion phenomena.









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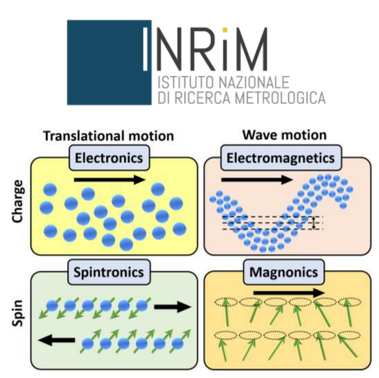
Magnetoelectric materials

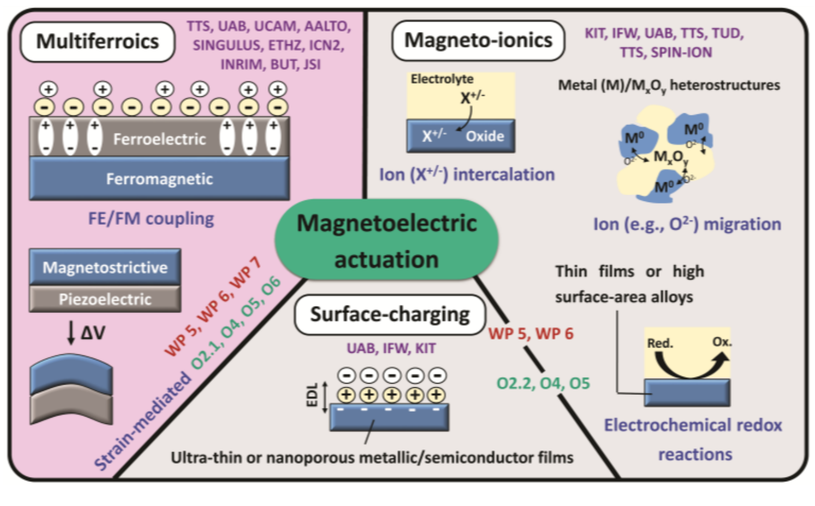
DESCRIPTION: in collaboration with INRIM BeMagic H2020 Project https://bemagic-etn.eu

OBJECTIVES: To develop new classes of energy-efficient spintronic devices for data storage systems

1) Growth of multiferroic structures by sputtering using top-down and bottom-up nanolithography to obtain small disks and other sub-micrometric geometries
2) Assessment of the magnetization properties

APPROACHES: Alloy synthesis by physical techniques, structural and microstructural characterisation (SEM, TEM, EDS, XRD, EBSD), measurement of magnetic properties. Work done in collaboration with a PhD student.





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