Finanziato dall'Unione europea
NextGenerationEU

Ministero dell'Università e della Ricerca

Italiadomani
PIANO NAZIONALE DI RIPRESA E RESILIENZA

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

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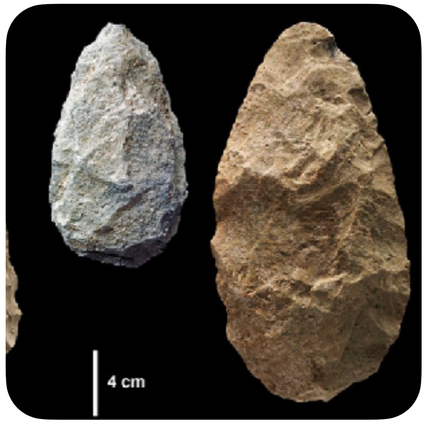
Spoke 7 – Materials and Molecular Sciences

Stefano Fabris - CNR

Kick off meeting 25/26 novembre 2022, Bologna



From the Stone to the Silicon Age

Materials Discovery
driven by the Digital Revolution

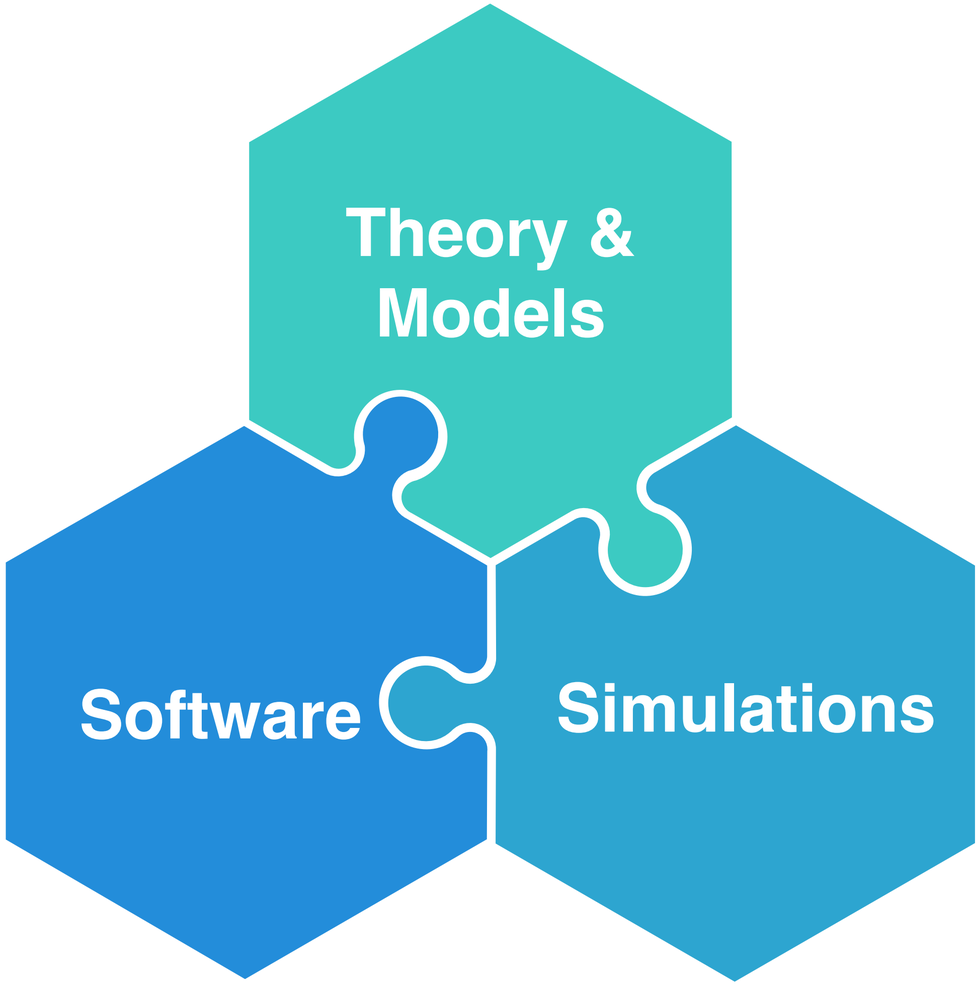
- Human civilisation has revolved around the discovery of new materials and of new functions for existing ones
- Energy, environmental and climatic emergencies, but also space economy or quantum technologies, ... our ability to face these challenges requires discovering new materials
- The complexity of challenges calls for a change of paradigm: It is no longer sufficient to hope to discover a material by chance
- Reverse engineering: properties for specific applications -> Design of novel materials

The Digital Revolution: HPC, Big Data, Quantum Computing

Materials Design & Discovery

- to solve the fundamental equations determining the properties of complex materials in realistic device condition

- to train artificial intelligence to predict complex emergent properties from databases



Goals & Objectives

Strengthen the Italian leadership in the development, implementation, maintenance, and free dissemination of software technologies for the multi-scale simulation of materials and molecular systems

Optimise existing HPC codes to stay at the leading edge of the main scientific, industrial, and societal challenges in the fields of materials and molecular sciences

Enable optimised access to the HPC infrastructure of the National Centre with emphasis on the transition to heterogeneous energy-savvy hardware architectures, aimed at exascale performance;

Promote competitiveness Steer the efforts of Italian materials and molecular modelling communities towards the key enabling technologies identified by the PNRR in conjunction with the private sector

Research Topics & Lines

WP1 Flagships Codes

Extension, optimisation, maintenance, and distribution of world-leading flagship codes for the high-performance numerical simulation of materials and molecular systems, developed by the national community

WP3 Accuracy&Reliability

Evaluation of the accuracy of the theory levels implemented in simulation codes with respect to the chemical accuracy standard

WP5 Materials Foundry

Development and enhancement of highly scalable, optimised codes/workflows towards an ecosystem of HPC applications for:

- Solving specific problems driven by industrial demands;
- Assisting and supporting experimental infrastructures and research

WP2 Big Data

Development and implementation of advanced methodologies for the generation and analysis of large volumes of data

WP4 Pilot Applications

Application of the software / middleware to solve selected and significant technological/scientific challenges, hitherto considered intractable

EuroHPC Joint Undertaking

Spoke program: in line and synergy with the with EU Open Software strategy and European HPC Joint Undertaking

11+1 participants

The Partnership

Leader
Consiglio Nazionale delle Ricerche CNR

Co-leader
SISSA

Affiliated members
Uni Trieste
Uni Trento
Uni Milano Bicocca
Uni Torino
Poli Torino
Uni Firenze
Uni Pisa
Uni Calabria
ENEA

Associated member
Uni Modena e Reggio Emilia -

Implementation

The Team

Staff

147
(89 with >3 PM/Y)

Recruitment

47
TD, AdR

PhD

15
2022/2023 – XXXVIII ciclo

11 October 2022 - CNR Headquarters

Kick off spoke 7

- Presentation of activities
- Definition of WP leaders
- Formation of working groups
- Appointment of spoke governance
- Project and budget timelines

Spoke Governance

Leader

S. Fabris - CNR

Co-leader

S. Baroni - SISSA

Spoke Assembly

M. Calandra - Uni Trento
F. Totti - Uni Firenze
B. Mennucci - Uni Pisa
L. Maschio - Uni Torino
D. Marchisio - Poli Torino
M. Celino - ENEA
M. Stener - Uni Trieste
M. Bernasconi - Uni MI Bicocca
S. Curcio - Uni Calabria

A. Ruini - Uni MoRe

Steering Committee

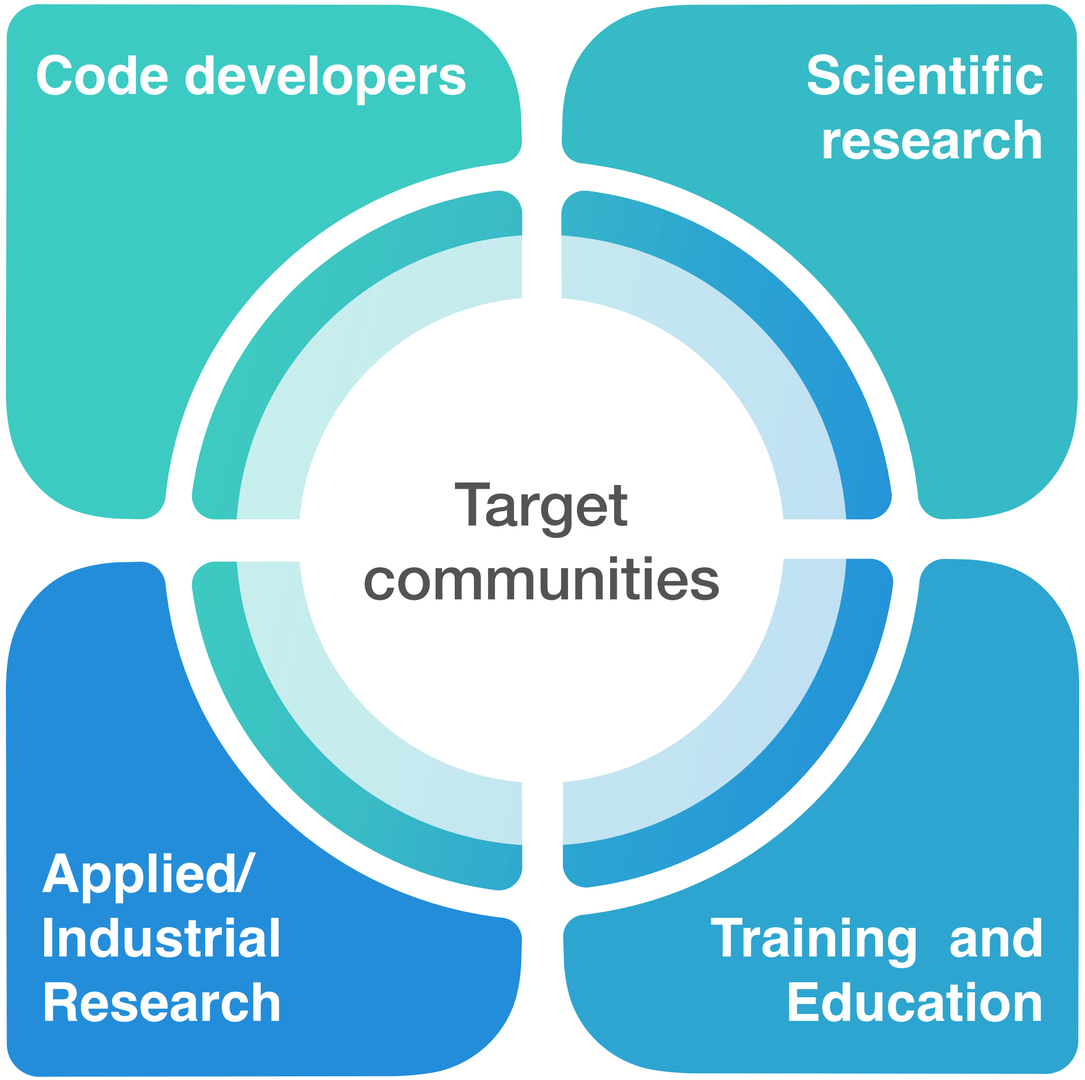
A. Ferretti, I. Carmineo - WP1
A. Marrazzo, G. Lattanzi - WP2
F. Lipparini, F. Santoro - WP3
A. Ruini, C. Di Valentin - WP4
A. Fortunelli, F. Dolcini - WP5

Technical secretariat

E. Narducci - CNR

Research

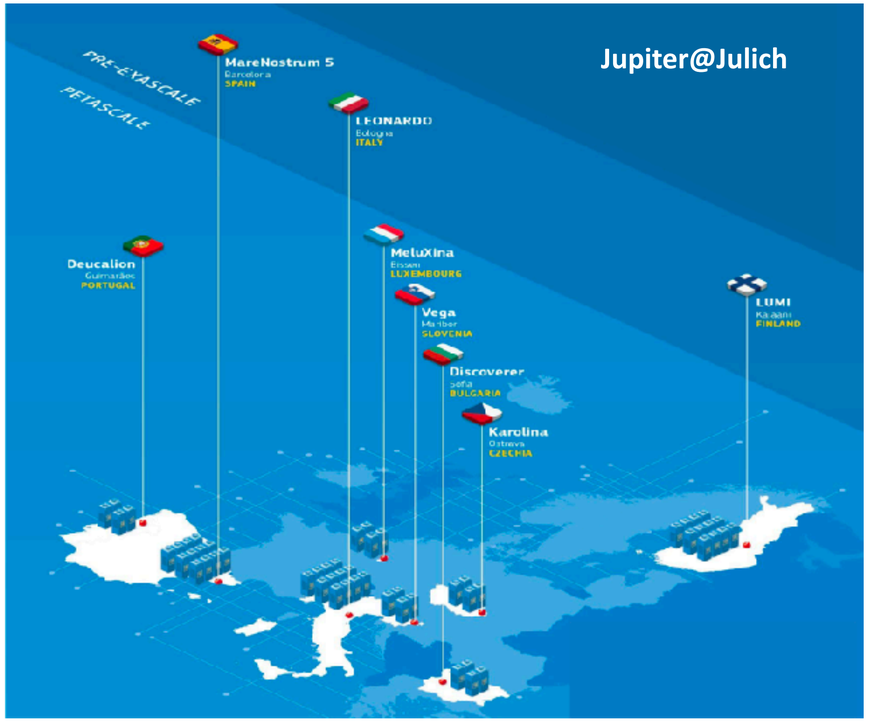
Methodology & Implementation



Research

WP1 Flagship codes

"WP1 will develop, maintain, and distribute CN flagship codes"



550 PFlops

240 PFlops

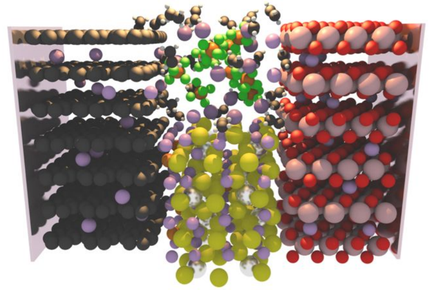
MareNostrum V

Exascale is (almost) here

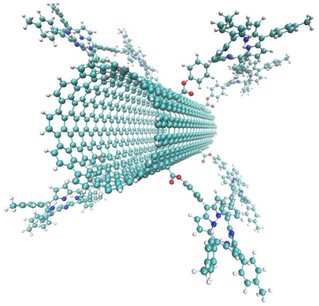
<u>SW Developments</u>

- To fully exploit the computational power available in HPC centers
- To treat large systems with accurate methods (e.g. large molecules, delocalized processes, low symmetry systems with large unit cells, longer time-evolutions);

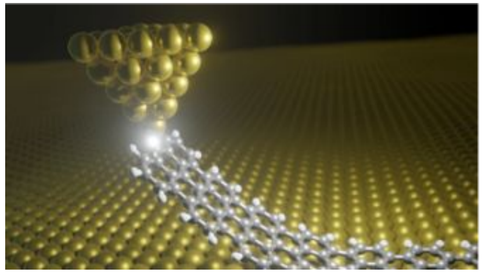
Lithium–ion batteries



Photo–induced processes

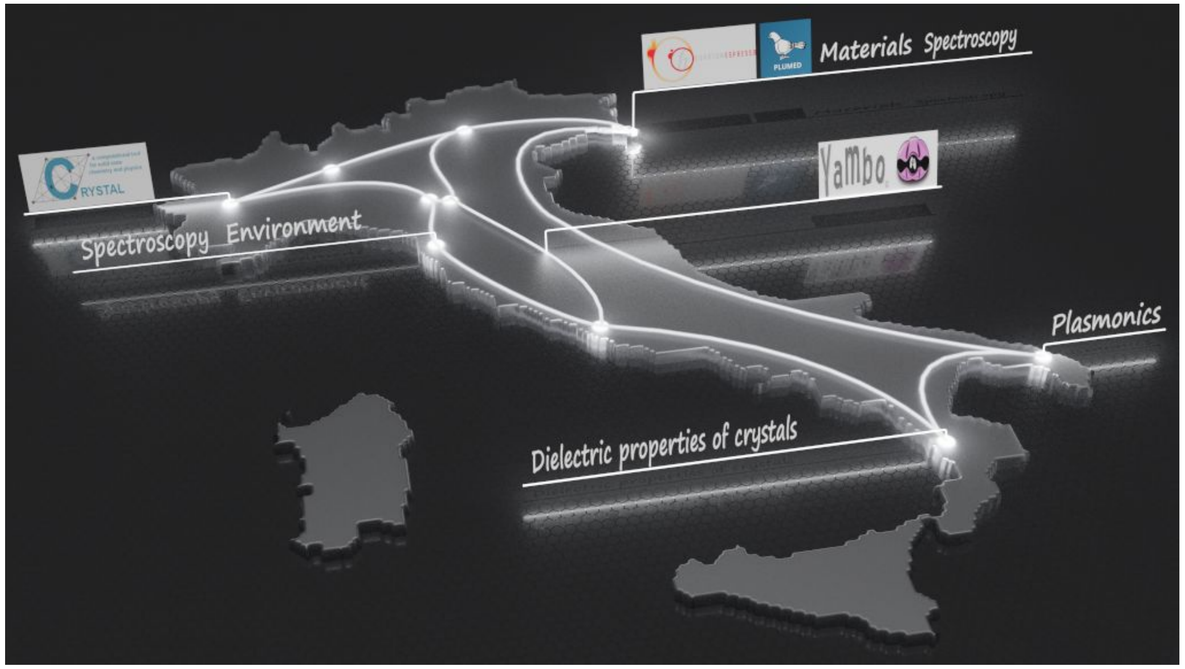


Electronic excitations at the nanoscale



WP1 Flagship codes

“WP1 will develop, maintain, and distribute CN flagship codes”



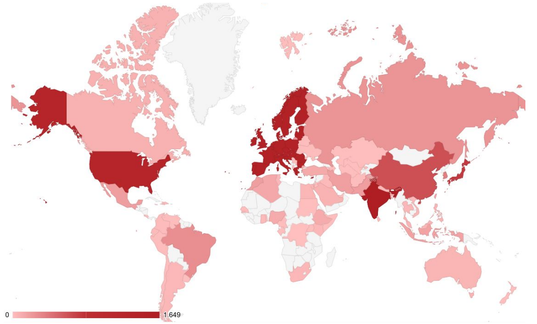
Flagship Codes

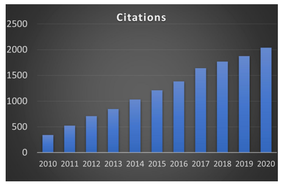
- To enhance the performance, portability and intra-node optimisation of the codes, including support of multiple GPU hardware (relevant in the EuroHPC context)
- To improve the parallel performance and scalability of the codes (especially addressing fast communications amongst accelerators)
- To enable long-term maintainability
- To implement new scientific features enabled by frontier HPC capabilities

WP1 Flagship codes

"WP1 will develop, maintain, and distribute CN flagship codes"

QUANTUM ESPRESSO™ is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials





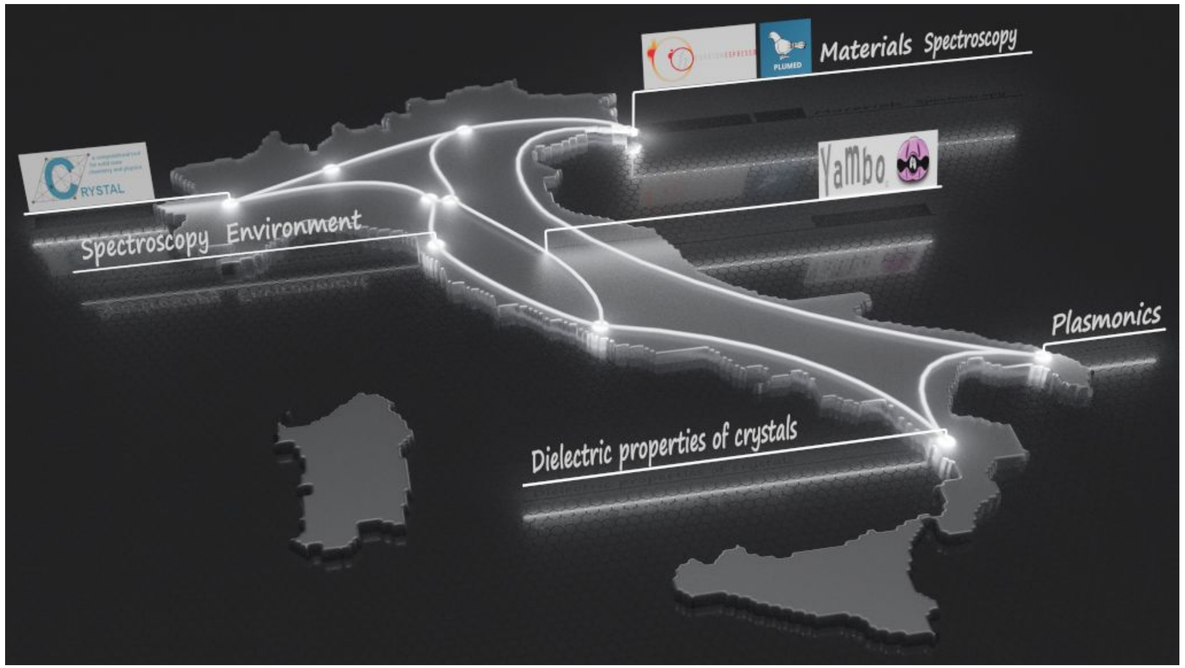
Yambo is an open-source code that implements many-body (post DFT) methods for finite and extended systems, with planewaves and pseudopotentials. Natively interfaced with QUANTUM ESPRESSO

The CRYSTAL package performs ab initio calculations of the ground state energy, energy gradient, electronic wave function and properties of periodic systems. It is a periodic ab initio code that uses a Gaussian-type basis set to express crystalline orbitals

PLUMED is an open-source, community-developed library that provides a wide range of different methods, which include: enhanced-sampling algorithms; free-energy methods; tools to analyze the vast amounts of data produced by molecular dynamics (MD) simulations.

WP1 Flagship codes

“WP1 will develop, maintain, and distribute CN flagship codes”



Flagship Codes

- …

Auxiliary Libraries

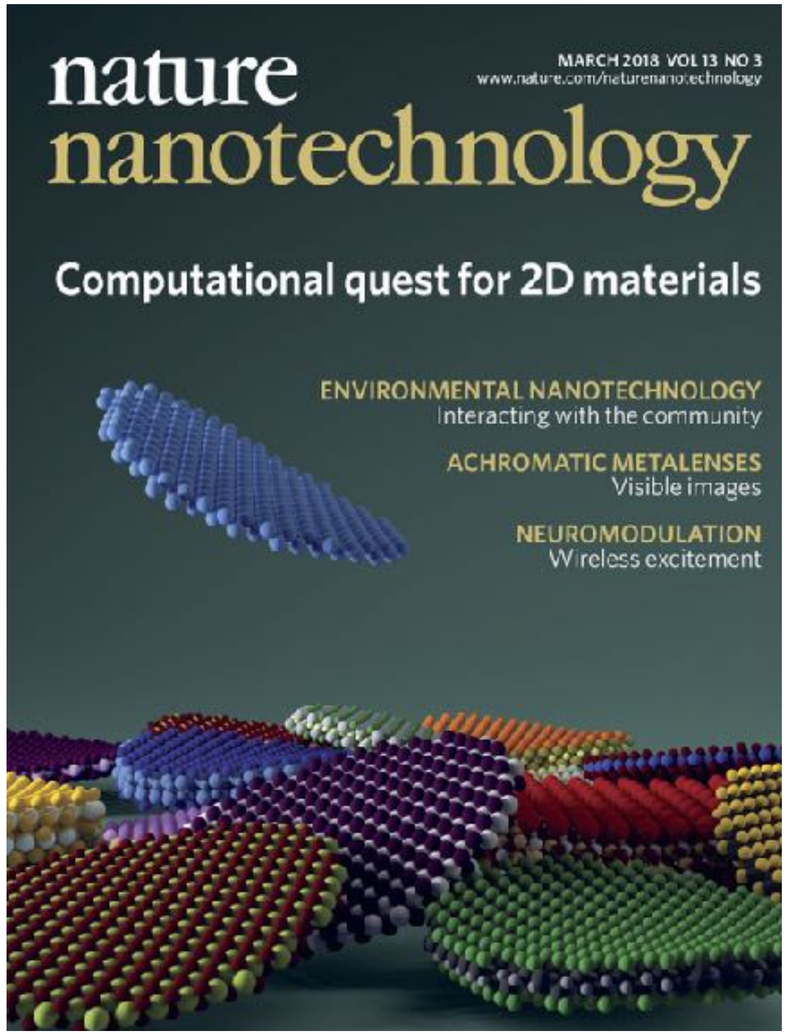
to perform specific high-level tasks, not bundled into any flagship codes

Materials Spectroscopy (ARPES, pump&probe, …)
Environment effects on materials properties (LibEnv, OpenMMPol)
Optical properties large systems (LibOpt)
Thermodynamic properties (ThermoPW)
Dielectric properties
Plasmonics (Turbomole)

Strong focus on exploiting current and emergent HPC architectures

WP2 Big Data generation and harnessing

Development of high-throughput computing, artificial intelligence, machine learning, and optimization techniques

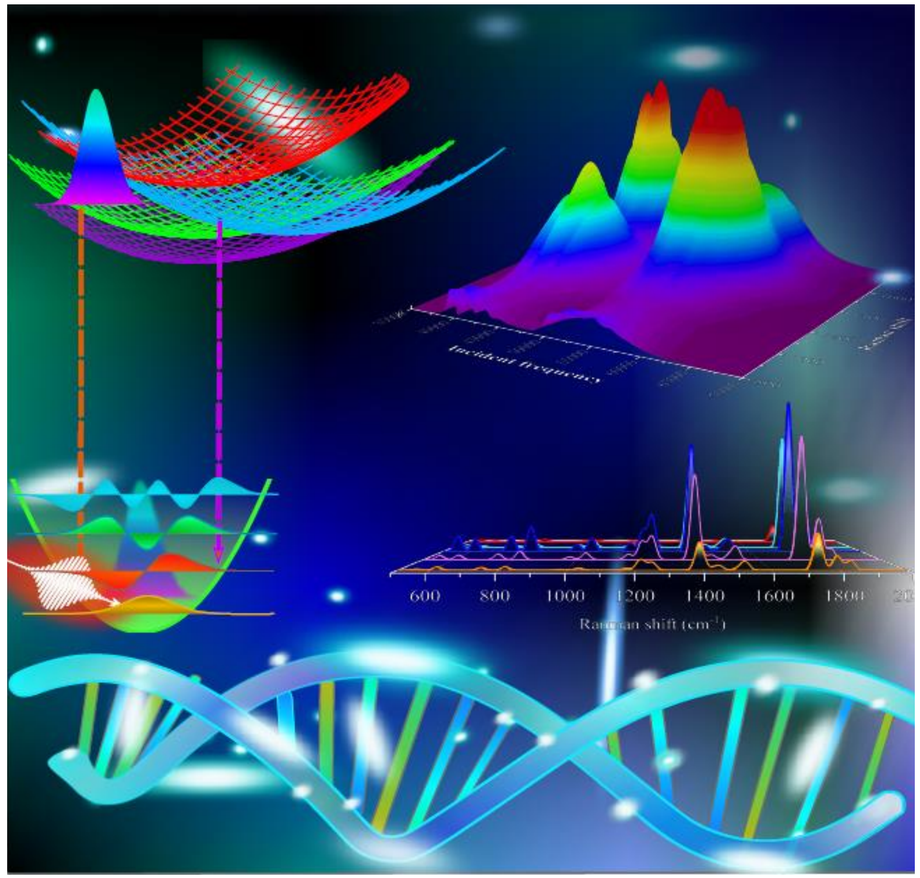


- discovery of new materials and drugs,
- development of predictive models of molecular interaction in complex systems

CODES	Fast generation of accurate data	**HPC**
Workflow middleware	Simulation management, data storage & retrieval	**HTC**
Data Analytics	Model extraction and reverse engineering	

WP3 Accuracy and Reliability

Evaluation of the accuracy of the theory levels implemented in simulation codes with respect to the chemical accuracy standard



QM and atomistic simulations relies on approximations

Validation of the energy functionals and diagrammatic expansions against accurate quantum-chemistry and quantum-Monte-Carlo data

Benchmarks

- accurate ground state calculations - DFT
- accurate excited state calculations- MBPT
- validation of interatomic potentials/force fields

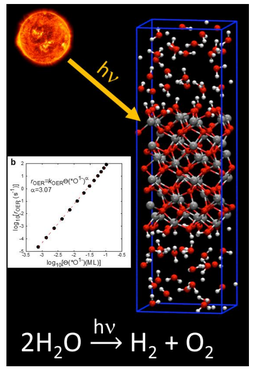
Research

WP4 Pilot applications

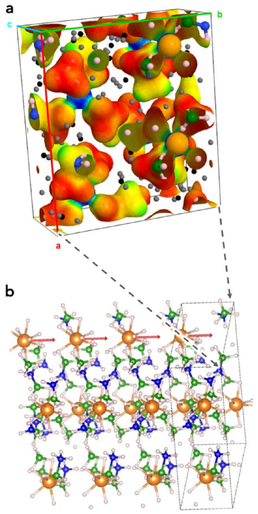
Validation of developed software and middleware against selected technological challenges

- WP4 will prove that outcomes of WP1 and WP2 satisfy end-users needs
- bridge with WP5 for specific applications of industrial and societal interest

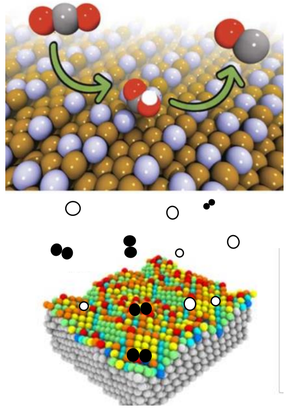
TASK 1 Simulation of physico-chemical processes controlling materials functions for ***energy applications***
TASK 2 Design and discovery of smart materials and systems for ***biomedical applications***
TASK 3 Complex systems for ***advanced technologies and applications***



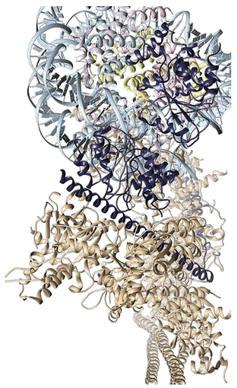
Photochemistry
And Solar fuels

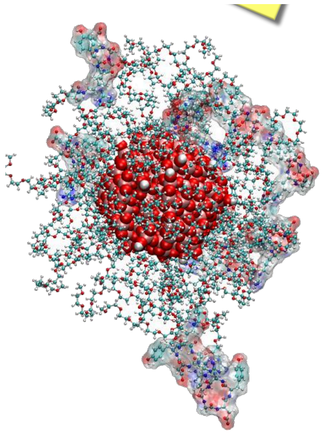


Batteries

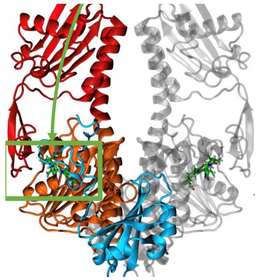


Fuel cells
and catalysis

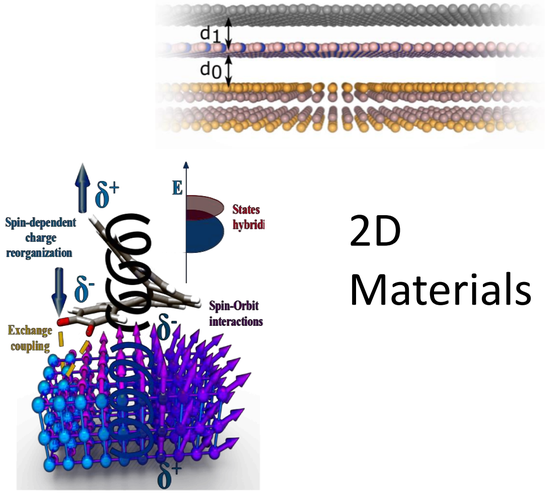




New Drugs &
Nano medicine



Photoreceptors



2D
Materials

Hybrid molecular
Materials

Research

WP5 Materials Foundry

rational design and discovery of new materials with tailored properties satisfying industrial demands and societal needs

D

Development

highly scalable, optimised codes and workflows towards an ***ecosystem of HPC applications***

I

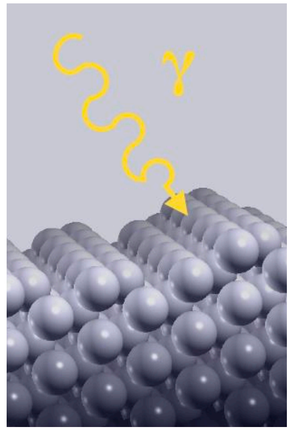
Industry & Private sector

Solving specific problems driven by industrial demands

E

Experimental facilities

Assisting and supporting experimental research and infrastructures
(synchrotron, neutron scattering, free-electron lasers)



Research

WP5 Materials Foundry

rational design and discovery of new materials with tailored properties satisfying industrial demands and societal needs

RESPONSE

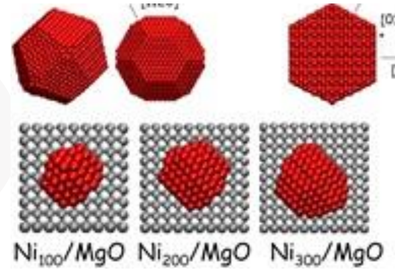
Simulation of spectroscopies, spectro- microscopy, diffraction, and scattering

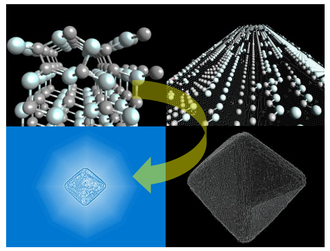
XPS, XRD, NMR, IR, XAS, Raman, ARPES, …

SAMPLING

Simulation of (micro)structure & dynamics, structure/response-property relationships

Activated/diffusive processes, phase/structural transitions, electron/mass transport,





MULTISCALE

structure & properties of complex materials in realistic environments

USER UPTAKE

enable a broad base of professionals without prior training to exploit the opportunities offered by materials and molecular modelling

Implementation

Technology Transfer

iFAB
INTERNATIONAL FOUNDATION
BIG DATA AND ARTIFICIAL INTELLIGENCE
FOR HUMAN DEVELOPMENT

Eni

LAVAZZA
TORINO, ITALIA, 1895

fater

SECO

Renewable Energy

Photovoltaics

Energy storage

Catalysis

Methods

Atomistic models and FF

Training on advanced simulation methods

Activated events

Reaction kinetics

Thermodynamics of materials/processes

Transport & diffusion

Automotive

Polymers

Innovation Funds/Open Call

Early 2023 - Industry workshop

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