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

Spoke 7 Materials & Molecular Sciences

Stefano Baroni & Stefano Fabris

Composizione dello Spoke

Leader

Consiglio Nazionale delle Ricerche CNR

Co-leader

SISSA

Membri affiliati

Uni Trieste

Uni Trento

Uni Milano Bicocca

Uni Torino

Poli Torino

Uni Firenze

Uni Pisa

Uni Calabria

ENEA

Membri Associati

Uni Modena e Reggio Emilia

Membri associati privati

ENI, Leonardo, IFAB.

Massa critica
148 unità di personale

Reclutamento
25 ricercatori tempo determinato
54 Assegni di Ricerca
29 Dottorati di ricerca

Facts & Figures

Programma scientifico su 5 WP

- Flagship Codes
- Big Data
- Accuracy and Reliability
- Pilot Applications
- Materials Foundry

Finanziamento totale
15.459.090,99 €

Partenariati pubblico-privati

- 6 progetti per l'innovazione
- 13 progetti bandi a cascata
- 14 aziende private
- 10 soggetti pubblici esterni

Produzione scientifica

- 5 codici di punta @exascale
- 2 codici HTC
- 7 workflows/applicazioni di AI/apprendimento automatico
- 2 codici potenziali interatomici su reti neurali (large scale)
- 17 codici/workflows per proprietà complesse di M&M

- 400+ pubblicazioni scientifiche su riviste internazionali
- 75+ software releases
- 1 conferenza di Spoke + conferenze, workshops, scuole
- Pilot projects and

Flagship codes

Ottimizzazione HPC di codici e librerie

- Esecuzione con successo di tutti i codici sul supercomputer Leonardo di CINECA (+ EuroHPC)
- Ottimizzazione e scalabilità avanzate su infrastrutture HPC di larga scala
- Porting su GPU per architetture eterogenee ad alte prestazioni
- Abilitazione multipiattaforma GPU (AMD, NVIDIA) per QE e YAMBO
- Costituzione di una solida rete naizonale di sviluppatori su codici flagship

QUANTUMESPRESSO

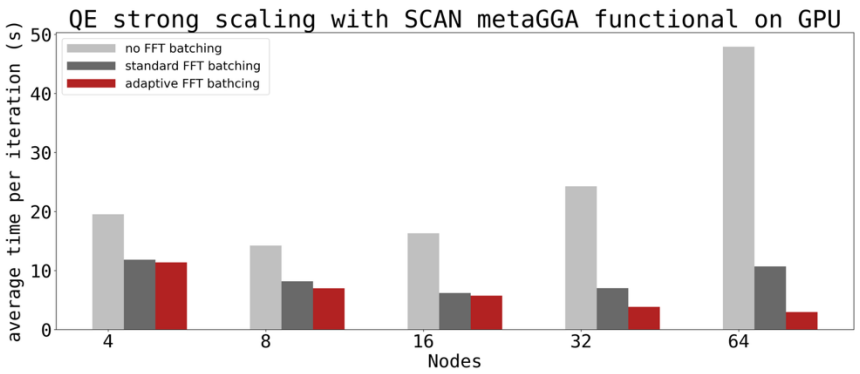
Yambo

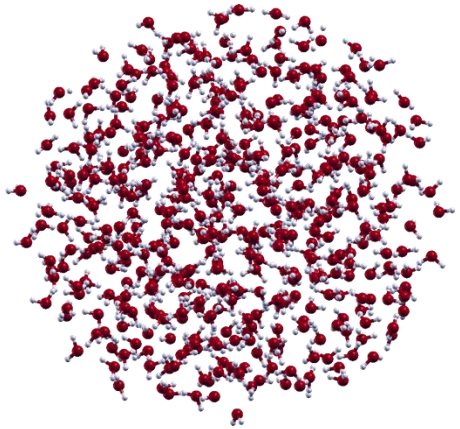
CRYSTAL a computational tool for solid state chemistry and physics

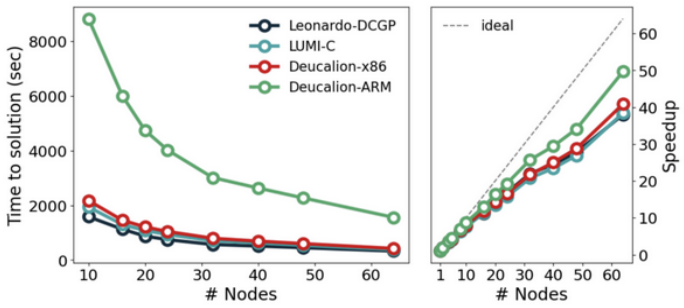
OpenMMPol

PLUMED

LibOpt



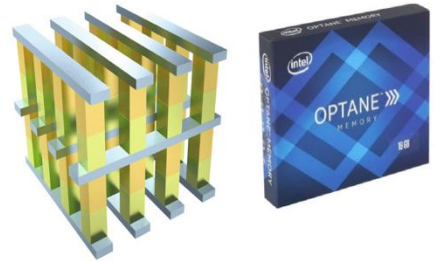


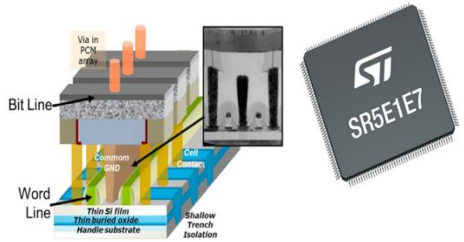


Big data generation and harnessing

Machine learning interatomic potentials for phase change materials

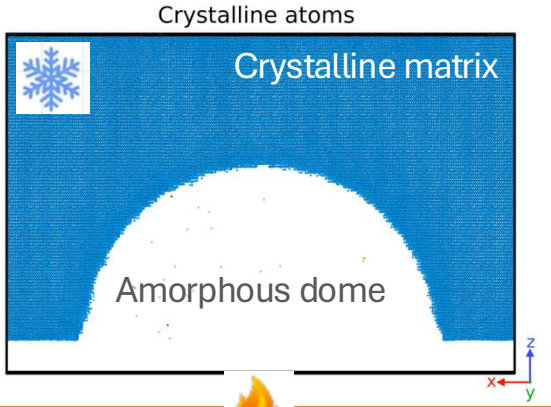
Phase change materials (GeSbTe alloys) are exploited in electronic non-volatile memories relying on the transformation between crystalline (metallic, bit 0) and amorphous (insulator, bit 1) phases upon heating





- Applications in standalone memory cards (Intel and Micron, 3D XPointTM); neuromorphic computing; embedded memories in microcontrollers (STMicroelectronics)

- **Achievement 1**: Generation of a MLIP for the flagship Ge2Sb2Te5 alloy
- **Achievement 2**: Unprecedented atomistic simulation of crystallization (set process) at real geometry (3 million atoms) and time scale (a few ns) of memory devices
- **Achievement 3**: Extention of MLIP to new Ge-rich GeSbTe alloys with higher crystallization temperature for applications in automotive



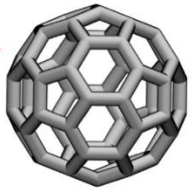
Pushing the accuracy of Electronic Structure Methods

Development of new algorithms for efficient Coupled Cluster Theory of large molecules

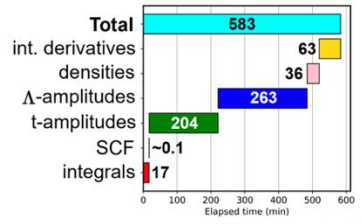
Pushing the limit of applicability of the accurate Coupled Cluster Theory to systems of direct technological interest

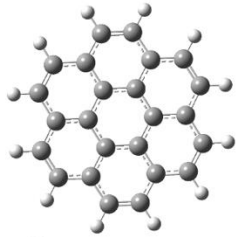
- **Technological relevance:** Robust implementation of LOBPCG and Davidson. Specialized algorithms for linear response equations. OpenSource (MPL)
- **Scientific relevance:** Coupled Cluster CCSD calculations and optimizations for large molecules are now possible
- **Contribution from ICSC activities:** Development of the algorithms and implementation in new freely available Libraries

New CCSD implementation
1800 basis functions
D_{2h} Symmetry
About 2h/iteration!



CCSD Geometry Optimization





900 basis functions

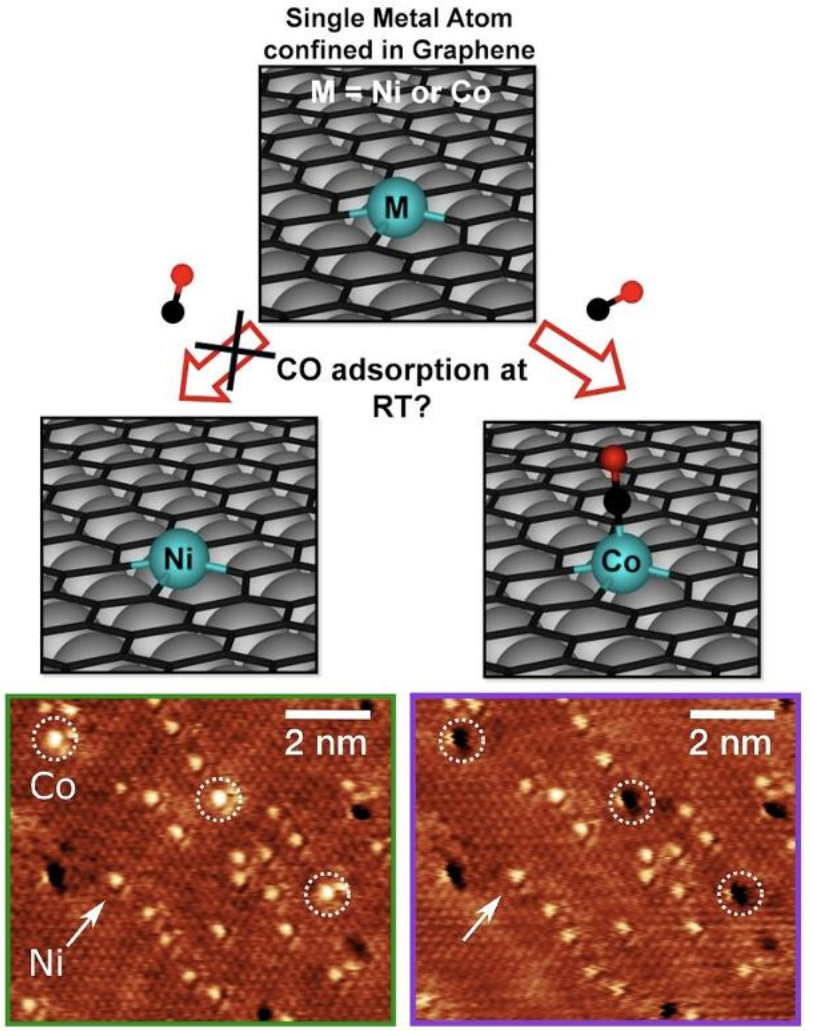
MOLECOLAB
diaglib
A COLLECTION OF MATRIX-FREE ITERATIVE EIGENSOLVERS

Metal Matters: Designing advanced catalysts

CO Adsorption on a Single-Atom Catalyst Stably Embedded i Graphene

Probe the reactivity of single metal atoms confined in graphene on Ni(111) using CO. At room temperature, CO binds to Co but not to Ni. Electronic analysis explains this selectivity, offering design principles for graphene-based single-atom catalysts.

- **Technological relevance:** Controlling CO adsorption on single atoms is key for catalysis and gas-sensing applications
- **Scientific relevance:** Ab initio modelling of chemisorption on functionalized graphene/Ni; electronic structure analysis and descriptors rationalize the selectivity. CO stretching frequencies computed to estimate the adsorption red-shif

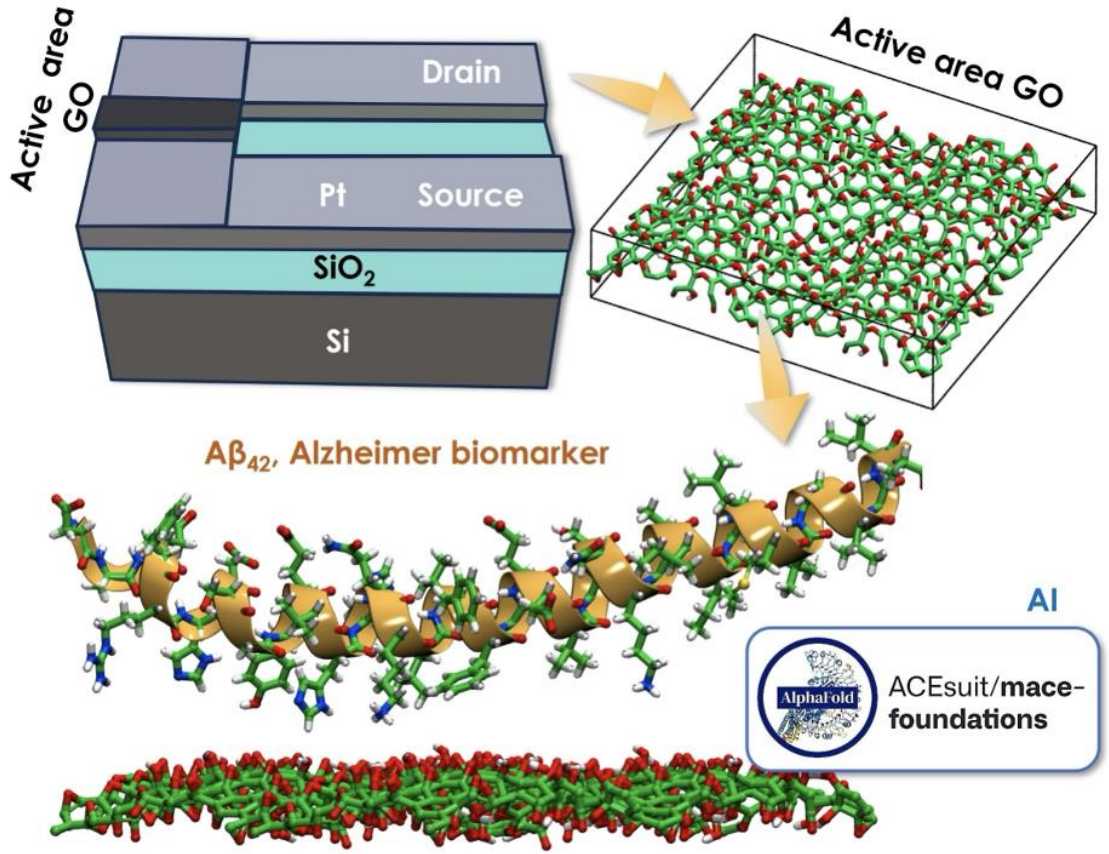


Advanced Bio-Sensors

Functionalized-Graphene Resistive Sensor for Alzheimer Detection

functionalized graphene oxide (GO) as the active area for detecting the Aβ42 protein, a key biomarker of the Alzheimer's disease (AD)

- **Technological relevance:** The sensor is promising for AD diagnostics from biological fluids, being extremely fast in response and selective toward Aβ42
- **Scientific relevance:** Modelling GO electro-optical properties via ab initio, explanation of main device characteristics from machine learning-based molecular simulations, involving proteins structural prediction and their interaction with the sensor



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