Theoretical Chemistry Group

From first principles to software implementation...

... through computers to the ab initio characterization of solids

Support & validate experimental works (Sinergic combination)

***In silico* experiments: Model system Theoretical model**

Prediction and interpretation of structure-property relationships

Expanding the modelling from small to very large systems

Theoretical Chemistry Group: Who

The scientific activity of the group mainly concerns the ***development*** ***and*** ***application*** ***of ab initio quantum-mechanical methods to solid state chemistry and physics and materials science***.

Silvia Casassa

Bartolomeo Civalleri

Marta Corno

Alessandro Erba

Anna M. Ferrari

Lorenzo Maschio

Piero Ugliengo

The group is one of the leading groups in the ab initio modeling of solids and materials and is actively collaborating with scientists from research centers and laboratories of both Italian and foreign universities

Theoretical Chemistry Group: What

Implementation *of QM methods and their* ***application*** *to solid state chemistry and materials science*

IMPLEMENTATION

Solid-state quantum mechanical computational tools

CRYSTAL — a computational tool for solid state chemistry and physics

www.crystal.unito.it

CRYSPLOT

A modern and easy to use visualization environment for plotting properties of crystalline solids as computed by means of the CRYSTAL code.

CRYSTAL VLAB

Molecular visualization software

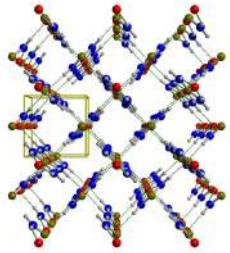
MOLDRAW

32-bit version

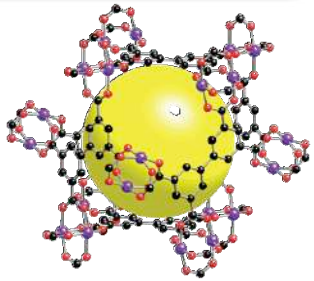
Display and manipulate molecules and crystals

INTERPLAY

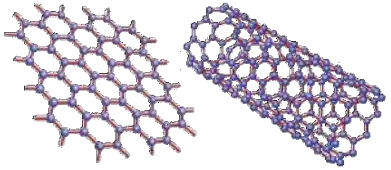
APPLICATION



Molecular crystals

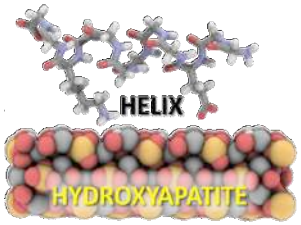


Metal-organic frameworks

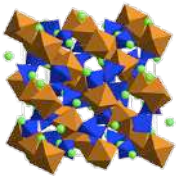


Nanomaterials

Hydrogen storage



Biomaterials



Minerals

Topic: Materials for 4th-generation All-Solid State Batteries

Supervisors: Lorenzo Maschio, Anna Maria Ferrari

Description: The new generation of solid state Li-ion batteries will allow for safer, cheaper and long-lasting batteries for automotive use

Objectives: to simulate properties of cathode materials (like NMC811, $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$) and new materials for solid state electrolyte (like $Li_{6.2}Ga_{0.1}La_3Zr_{1.5}Bi_{0.5}O_{12}$ and their interface. Such properties include thermal expansion, Li-ion diffusion coefficients and mechanical stresses following Lithium mobility.

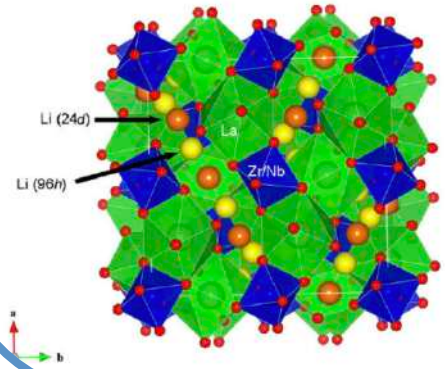
In Collaboration with:

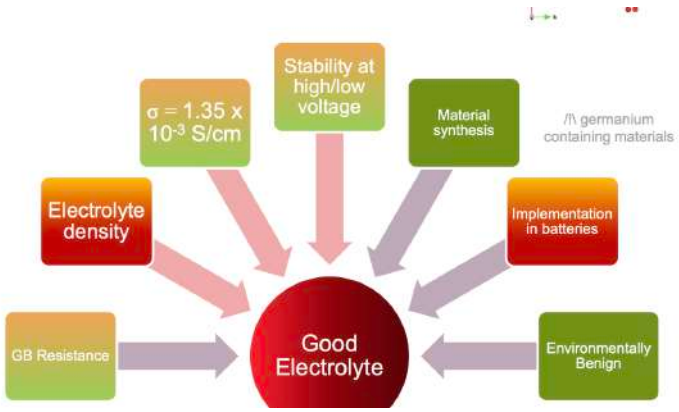
CRF

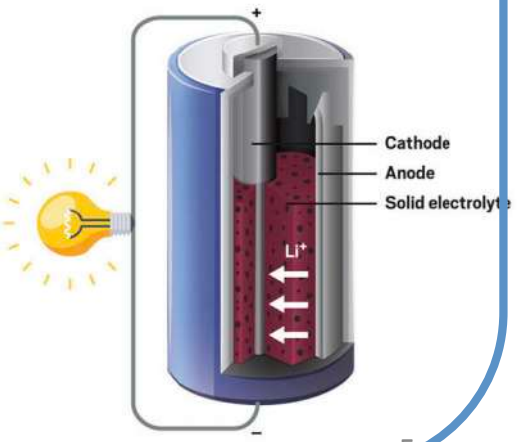
gemmate technologies

MODALIS 2

Approaches: quantum-chemical ab initio simulations using the CRYSTAL code.



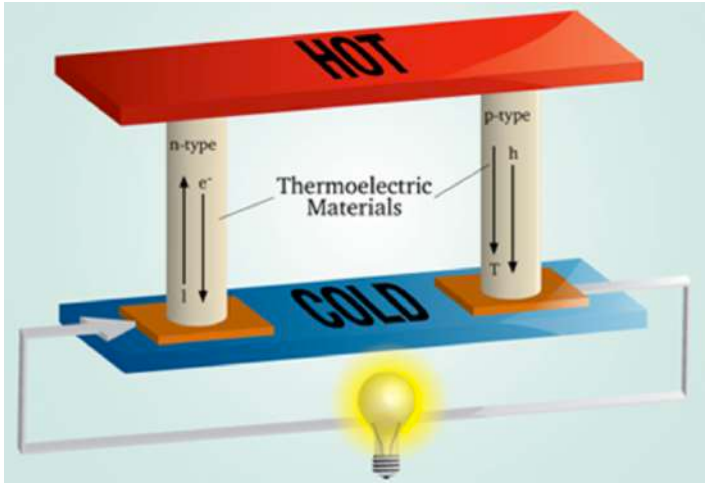


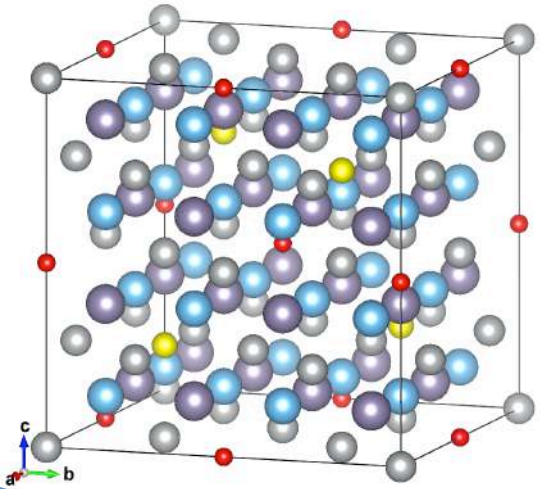


Topic: Thermoelectric Materials from Ab Initio Calculations

Supervisors: Lorenzo Maschio, Silvia Casassa

Description: Thermoelectrics are among the most interesting new materials, since they allow to convert temperature gradients (like waste heat) into useful electricity. The challenge is to design materials that are cheap, efficient and environmentally friendly. In this respect, simulation can be very useful, allowing to select potentially interesting structures before synthesizing them, and helping in the understanding of the underlying physical phenomena





Objectives: to simulate properties of thermoelectric materials like TiNiSn and other Half-Heusler alloys, elucidating the role of defects in their thermoelectric and electron transport properties

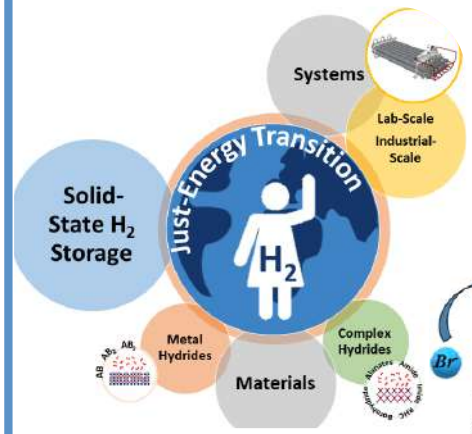
Approaches: quantum-chemical ab initio simulations using the CRYSTAL code.

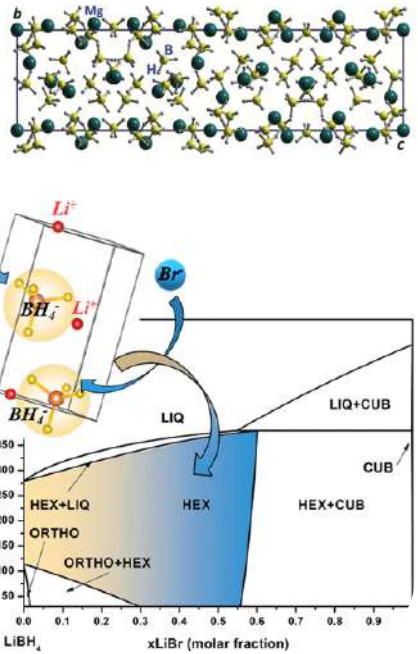
Topic: **Modelling of advanced materials**

Supervisors: Marta Corno

ENERGY MATERIALS

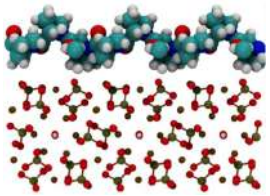
- ✓ $LiBH_4$-based electrolytes for all-solid-state Li-ion **batteries**
- ✓ Solid-state carriers for **hydrogen storage**

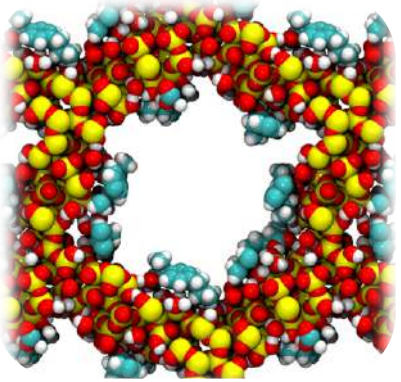




BIOMATERIALS

- ✓ **Drug delivery systems**, mainly silica based materials and nanosponges
- ✓ **Nano bio-interfaces for bone implants**, mainly hydroxyapatite + collagen + water





Ibuprofen in mesoporous silica

Melatonin in β-cyclodextrin

Topic: Weak interactions in solids: from molecular crystals to porous materials

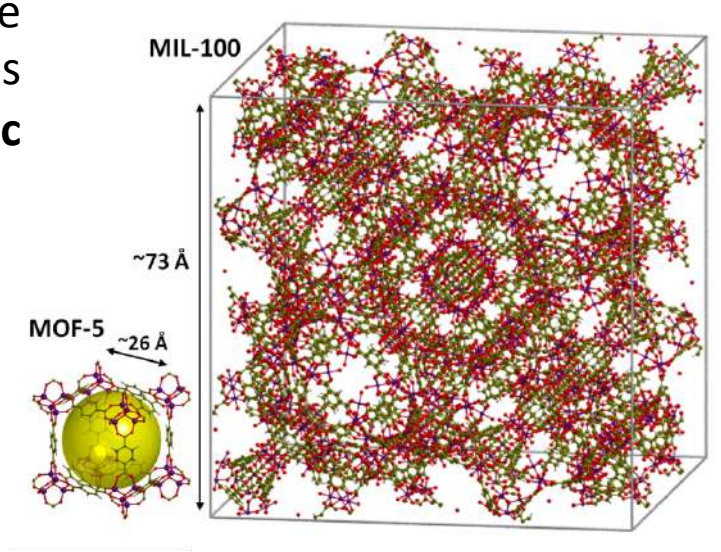
Supervisors: Bartolomeo Civalleri

Description:

• Implementation and validation of DFT-based methods for the study of **weak interactions in solids** with application to molecular crystals and adsorption in porous materials.

• Interaction of small (e.g. CO_2 capture) and large molecules (e.g. drug delivery, pollutants removal) in the pores of **Metal-Organic Framework materials**.

• Development of **cost-effective composite** electronic structure **methods** for solid state calculations



Approaches: quantum-chemical ab initio simulations using the CRYSTAL code.