DRIVING
THE EXASCALE
TRANSITION

Materials design At the eXascale

European Center of Excellence for HPC applications
an H2020 e-infrastructure

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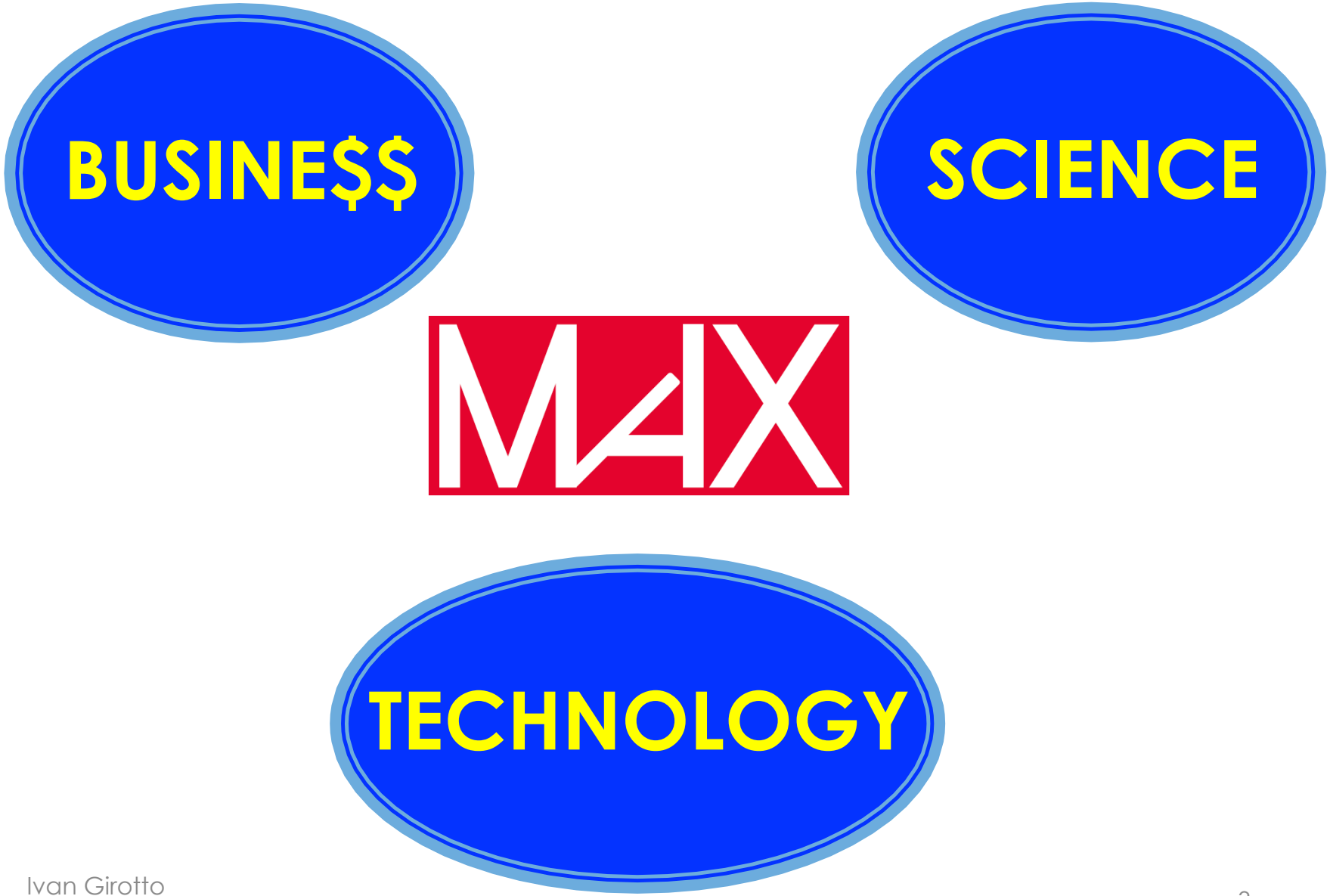
Information & Communication Technology Section (ICTS)
International Centre for Theoretical Physics (ICTP)

… a Centre of Excellence in materials modelling, simulations, and design able to unleash the EU leadership in this field and in high-performance computing

and **to empower our core communities** with powerful new instruments to address the key scientific, industrial and societal challenges that require novel materials.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fleur

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AiiDA
Automated Interactive Infrastructure and Database for Computational Science

SCIENCE

MAX

siesta

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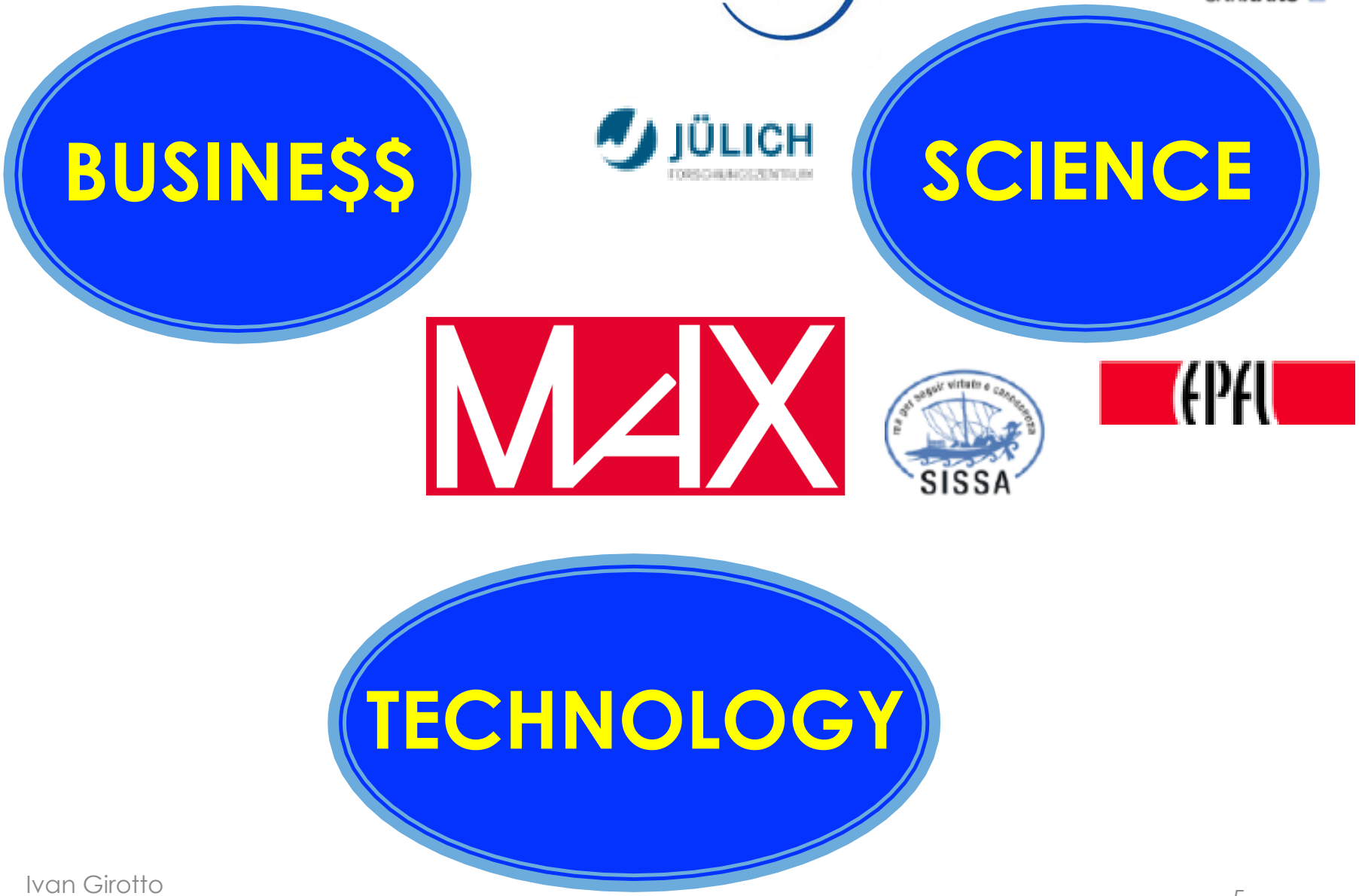
TECHNOLOGY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MAX

E4 COMPUTER ENGINEERING

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JÜLICH

SISSA

Principal Investigators

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Coordinator

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SISSA (IT)

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EPFL (CH)

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Cloudweavers Ltd (UK)

Prof. Erwin Laure

KTH (SE)

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E4 (IT)

Dr. Ivan Girotto

UNESCO-ICTP (IT)

action lines

1. **creating an ecosystem of capabilities, applications, data workflows and analysis: needed now, and ready for the exascale**
2. **training, dissemination, industry**

action lines

1. creating an ecosystem of capabilities, applications, data workflows and analysis: needed now, and ready for the exascale

- community **codes** for quantum simulations:
  their capabilities and reliability
- transition to **exascale** architectures,
  energy awareness, codesign, …
- **workflows**; **data** provenance, preservation, sharing and analytics
- an **ecosystem** that integrates capabilities, available
  to researchers in academia and industry
- a set of pilot cases: **excellent science of direct industrial relevance**

action lines

2. training, dissemination, industry

- key **services to the core communities**:

  codes, data, expertise, training

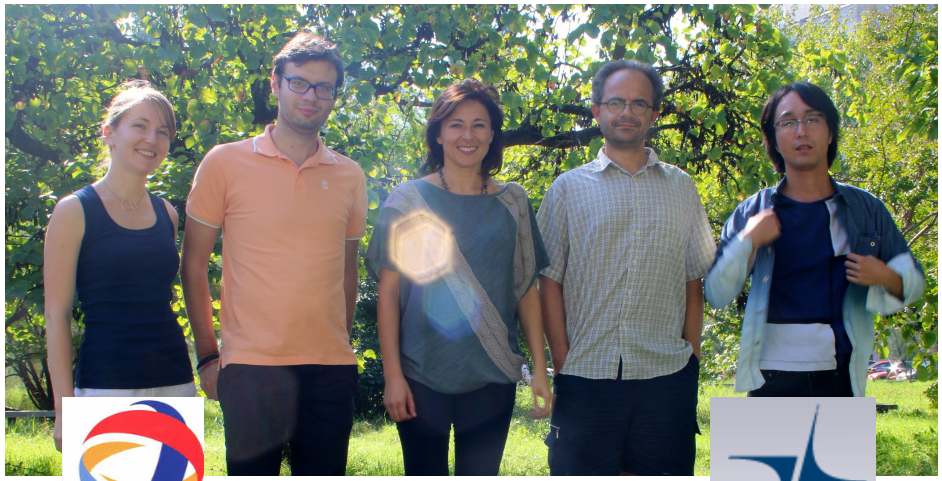
- **training**: coordination, integration, access
- **turn-key solutions for end users in research and industry**, incl. SMEs:

  build a ‘market place’ starting from our pilots, outreach

Pilot case 1: M.C. Righi (Cnr Modena)
Computational protocol for friction and tribochemistry

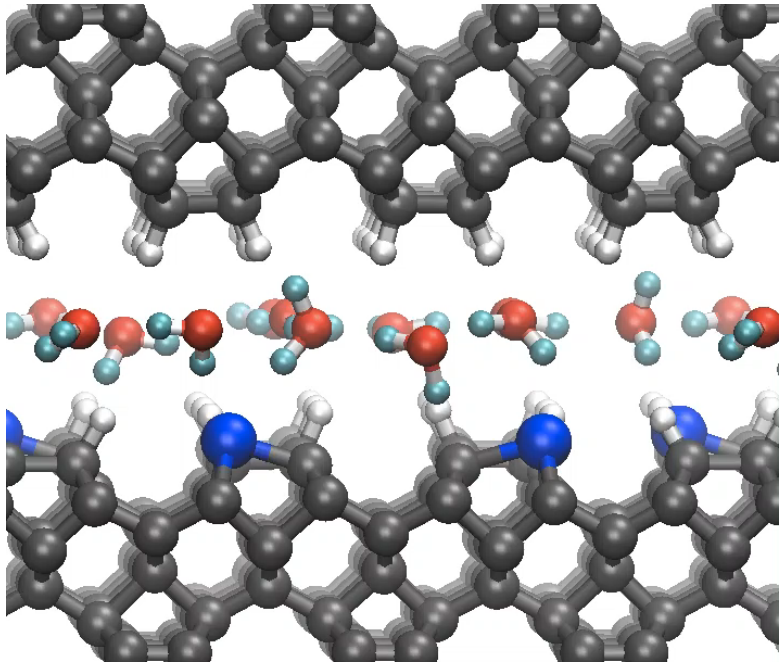
Goal: controlling friction through materials design → coatings, lubricants (in collab with Toyota and Total)

Problem: enhanced reactivity, classical MD not enough → computational tribochemistry incl. quantum effects



TOTAL

Toyota CLabs



Strategy: Ab initio mol. dynamics based on modified versions of Born Oppenheimer MD + Car Parrinello cp.x computer code

Deliver:

- workflow: MD tribochemistry simulations
- automated procedures & database
- training through research in MaX labs

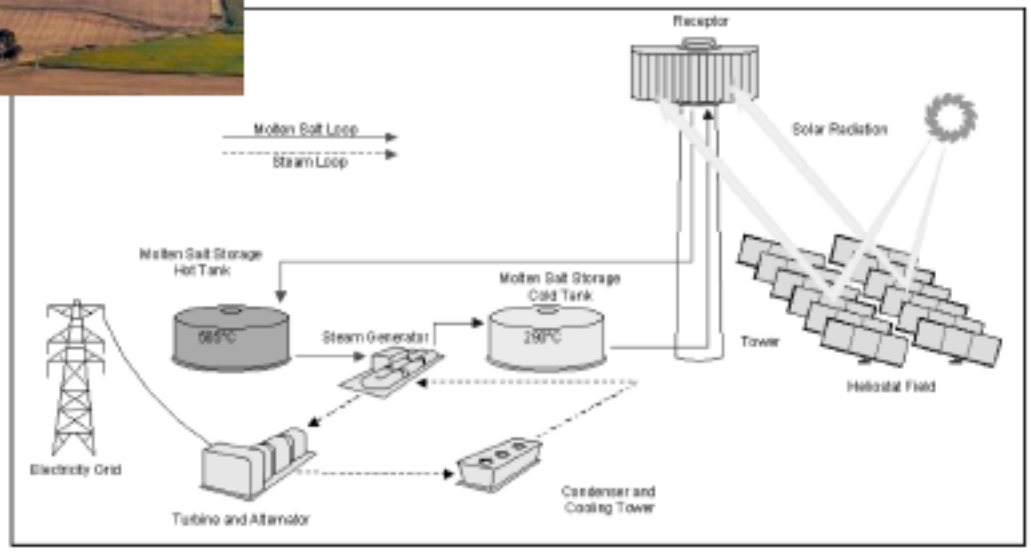
Pilot case 2: P. Ordejón (ICN2)
Computational protocol for understanding thermal storage in molten salts and nanofluids

ABENGOA

Innovative technology solutions for sustainability

Molten salts:

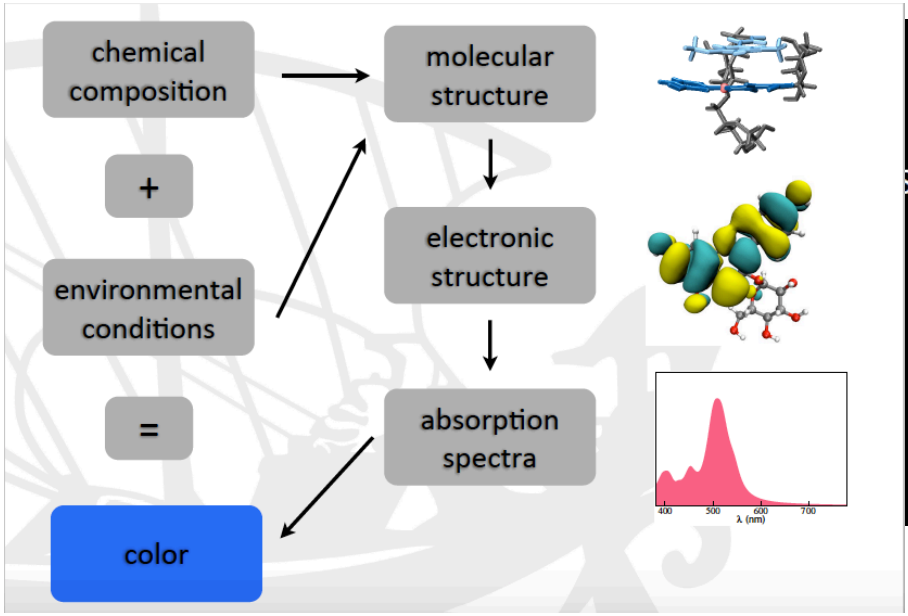
- Heat storage and transport medium
- Allow electric energy generation in the absence of sunlight (with heat stored during daylight)
- Melting: ~200ºC
- Operation: ~500ºC
- High heat capacity

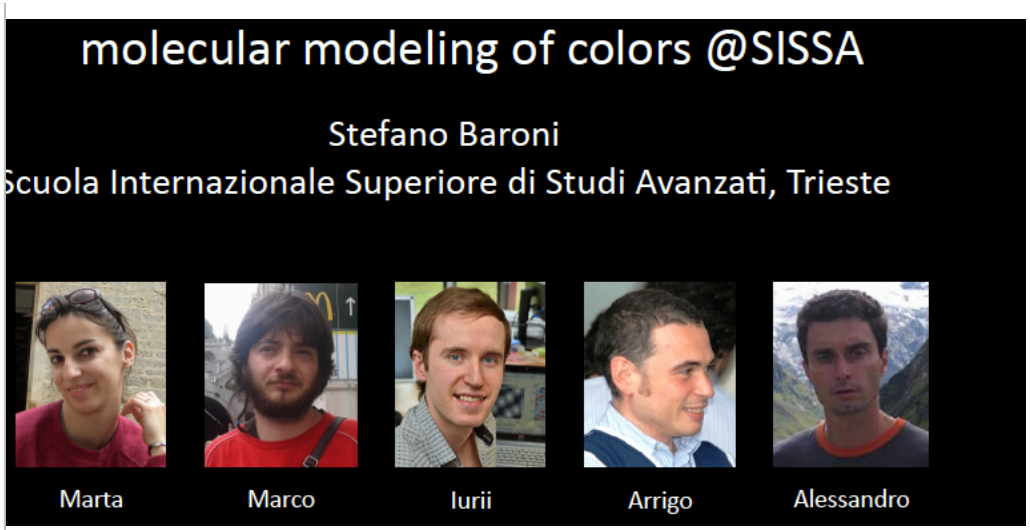


Pilot case 3: S. Baroni(SISSA)
Computational protocol for simulating the color optical properties of natural dyes for food industry applications

- study and understand the properties of the colors
- replace synthetic colorants with natural colorants

MARS incorporated





Pilot case 4: N. Marzari(EPFL)
Design and discovery of optimal solid-state electrolytes

The search for novel Lithium-ion conductors

Motivation:

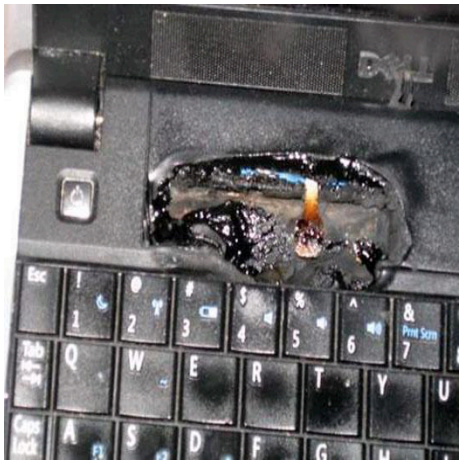
- Safety of current systems
- Increase performance
- Enable high-voltage

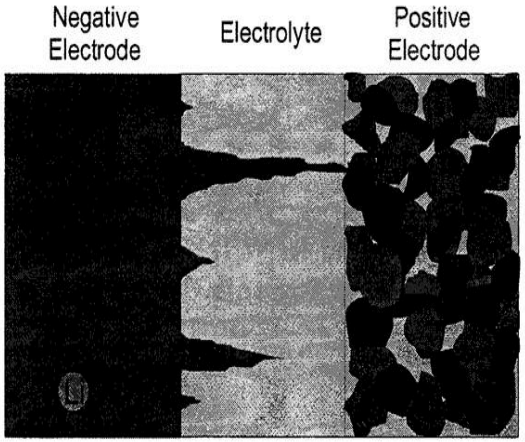
Key objectives:

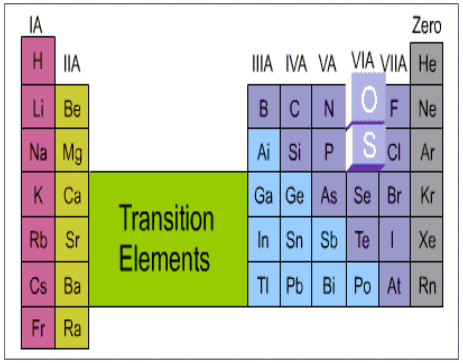
- Find candidates for electrolyte in solid-state lithium-ion batteries
- Find descriptors of ionic conductivity

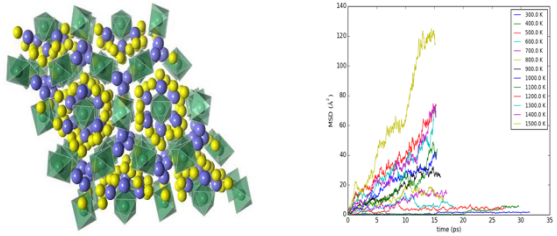
Approach:

- 1207 structures (containing O, Li, insulating) from database
- 2264 deriving structures
- BOMD simulation from first-principles at 3 temperatures
- Analysis









Descriptors

BOSCH
Invented for life

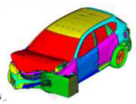
GLOBAL CONTEXT: *Increasing Recognition of Impact of HPC Enabled Applications*

U.S. President Barack Obama issued an executive order establishing the National Strategic Computing Initiative with initial allocation of $ 450 M from the U.S. Department of Energy). (29/07/2015)

Former Vice President of the European Commission Neelie Kroes announced the launch of a contractual Public-Private Partnership (cPPP) on Big Data (€ 500M EC funding) and for the development of a European HPC Eco-system (€ 700 M EC funding). (17/12/2013)

French President François Hollande announced the launch of French National "Plan Supercalculateur" with € 50M of national funding. (07/05/2014)

Chinese President Xi applauds success of world's fastest supercomputer Tianhe-2 built by China's National University of Defense Technology with the fundamental purpose of *"providing a driving force for the construction of an innovation-oriented country"*. (18/06/2013)

Category	Priority issues
Enhancement of industrial competitiveness 	⑦ **Creation of new functional devices and high-performance materials to support next-generation industries** Accelerate the development of electronics technologies, structural materials, functional chemical products etc. that have great international competitiveness, through coordination with large-scale massively parallel computing and the analysis of "Big Data" and data from measurement and experimentation, in order to create devices and materials to support next-generation industries. 
	⑧ **Development of Innovative Design and Production Processes that Lead the Way for the Manufacturing Industry in the Near Future**

Social and scientific priority issues to be tackled by using Post 'K' Computer(1

. Priority issues（9 issues）

・We selected nine social and scientific priority issues from the following point of view;

(1) High priority issues from a social and national viewpoint
(2) Promising Creation of World-Leading achievement
(3) Promising Strategic Use of Post 'K' computer

Executive Order
Creating a National Strategic Computing Initiative

[…]
This coordinated research, development, and deployment strategy will draw on the strengths of departments and agencies to move the Federal government into a position that sharpens, develops, and streamlines a wide range of **new 21st century applications**. It is designed to advance core technologies to solve difficult computational problems and foster increased use of the new capabilities in the public and private sectors.

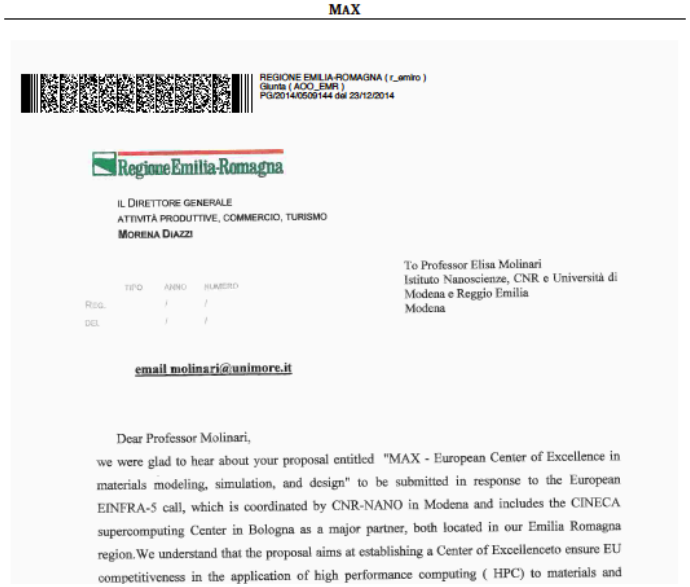
[…]
It is also important to note that HPC in this context is not just about the speed of the computing device itself. […] **HPC "must now assume a broader meaning, encompassing not only flops, but also the ability, for example, to efficiently manipulate vast and rapidly increasing quantities of both numerical and non-numerical data."**

over the next decade HPC systems are expected to be capable of
one **exaflop** (10^{18} operations per second) and
to manage and analyse data sets up to one **exabyte** (10^{18} bytes)

Conclusion and Acknowledgements

- In 2014-2015 EU founded the EINFRA5 for ~ 37.5M euros
- About 4M were awarded to intalian Insitutions (0.8M to the Trieste area)
- About 1.8M were awarded to the MaX project

*data provided by APRE (TS)



MAX

REGIONE EMILIA-ROMAGNA (r_emiro)
Giunta (AOO_EMR)
PG/2014/0509144 del 23/12/2014

Regione Emilia-Romagna

IL DIRETTORE GENERALE
ATTIVITÀ PRODUTTIVE, COMMERCIO, TURISMO
MORENA DIAZZI

TIPO ANNO NUMERO
REG. / /
DEL / /

To Professor Elisa Molinari
Istituto Nanoscienze, CNR e Università di
Modena e Reggio Emilia
Modena

email molinari@unimore.it

Dear Professor Molinari,

we were glad to hear about your proposal entitled "MAX - European Center of Excellence in materials modeling, simulation, and design" to be submitted in response to the European EINFRA-5 call, which is coordinated by CNR-NANO in Modena and includes the CINECA supercomputing Center in Bologna as a major partner, both located in our Emilia Romagna region. We understand that the proposal aims at establishing a Center of Excellenceto ensure EU competitiveness in the application of high performance computing (HPC) to materials and

MAX

REGIONE AUTONOMA
FRIULI VENEZIA GIULIA

l'Assessore regionale al lavoro, formazione, istruzione, pari opportunità, politiche giovanili e ricerca

tel + 39 040 377 5172
fax + 39 040 377 5176
assessorelavoro@regione.fvg.it
I - 34133 Trieste, via San Francesco 37

Trieste, January 9th 2015
Protocollo n. 1/S.P./F-2b

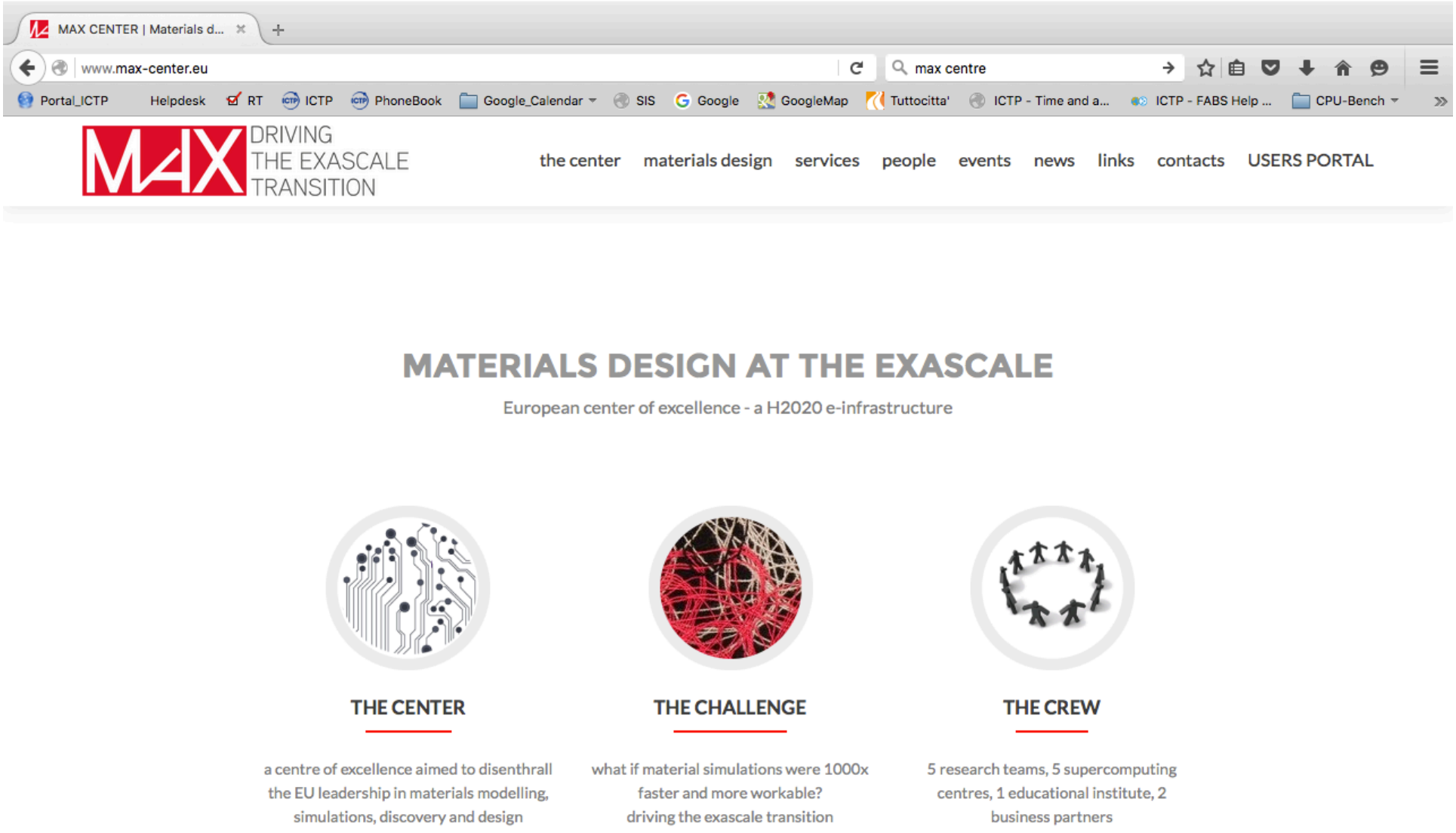
To
Prof. Elisa Molinari
Istituto CNR-NANO ed Università di Modena e
Reggio Emilia
Modena

Director professor Guido Martinelli
Professor Stefano Baroni
SISSA (International School for Advanced Studies)
via Bonomea 265
34136 Trieste – Italy

Letter of endorsement

We - the Regional Authority of Friuli Venezia Giulia, Central Directorate for Job, Training, Education, Equal Opportunities, Youth Policies and Research - recognize that the project entitled "MAX - European Center of Excellence in materials modeling, simulation, and design", to be submitted in response to the European EINFRA-5 call connected to Horizon 2020, is of great interest for the Region Friuli Venezia Giulia for the strategic importance of the proposal, the probable impact of the research and the potential achievement of a significant progress in knowledge in this scientific field, not only with regard to the scientific and academic system but also for the probable outcomes on a socio-economic level.

For these reasons, we're very glad to support the proposal "MAX", which includes SISSA as a member of the composite partnership, coordinated by Professor Elisa Molinari, CNR-NANO in Modena. In particular, we appreciate the fact that the initiative aims at establishing a Center of Excellence in the application of high performance computing (HPC) to materials and nanotechnologies, placing computational science and the harnessing of 'big data' at the center of



www.max-center.eu