PaNOSC status update:

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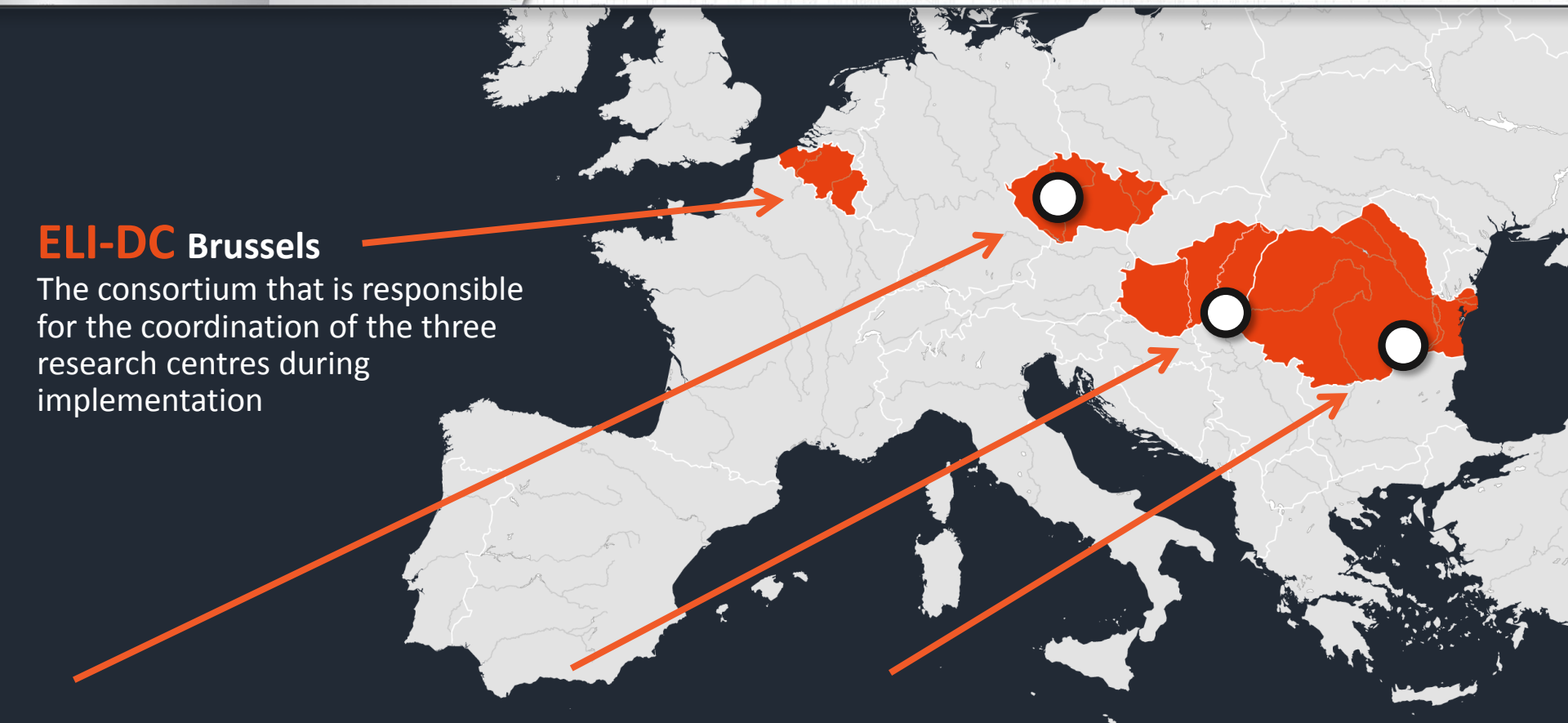
Computational Materials Research, Theory & Simulation

ELI-ALPS, Szeged, Hungary

WP5 development sprint
20th to 30th April, 2020

SZÉCHENYI 2020
HUNGARIAN GOVERNMENT
European Union
European Regional Development Fund
INVESTING IN YOUR FUTURE

The Research Institutes (sites) of ELI



ELI-DC **Brussels**
The consortium that is responsible for the coordination of the three research centres during implementation

ELI-BL **Dolny Brezany**
Czech Republic
Ultrashort x-ray generation, particle acceleration

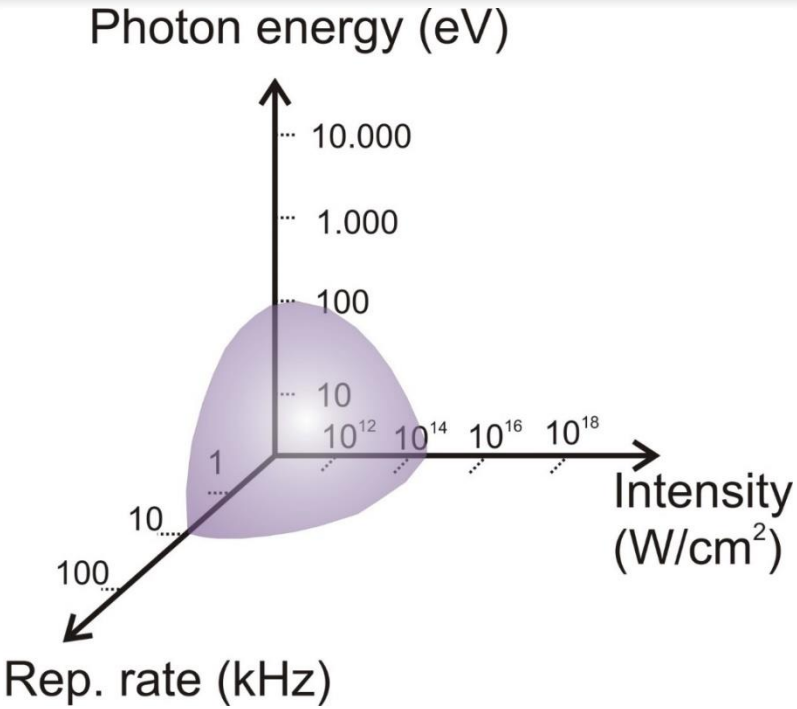
ELI-ALPS **Szeged**
Hungary
Ultrashort laser pulses at high repetition rate

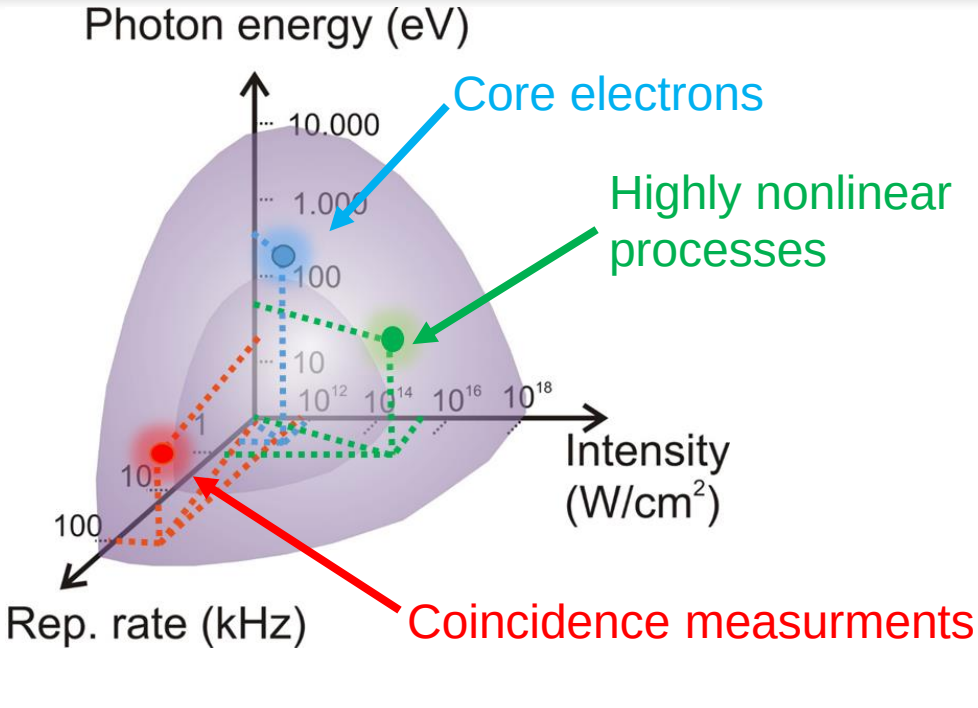
ELI-NP **Magurele**
Romania
Ultra-intense optical and gamma ray pulses

UHFS
Ultra-High-Field Science
unprecedented laser field strength
(location: TBD)

Activity range at ELI-ALPS

ELI-ALPS user facility





1) Generation of XUV/X-ray femto- and attosecond pulses
   → Attosecond scale of electron dynamics in atoms, molecules, plasmas and solids

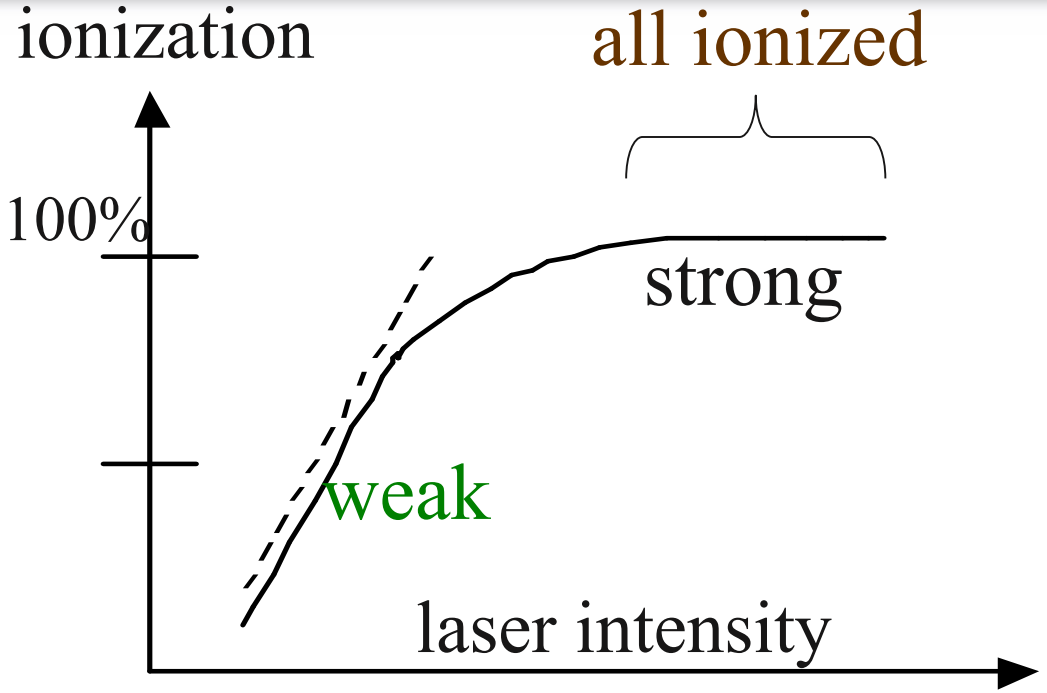
ATTOSECOND Beamlines & User Facility

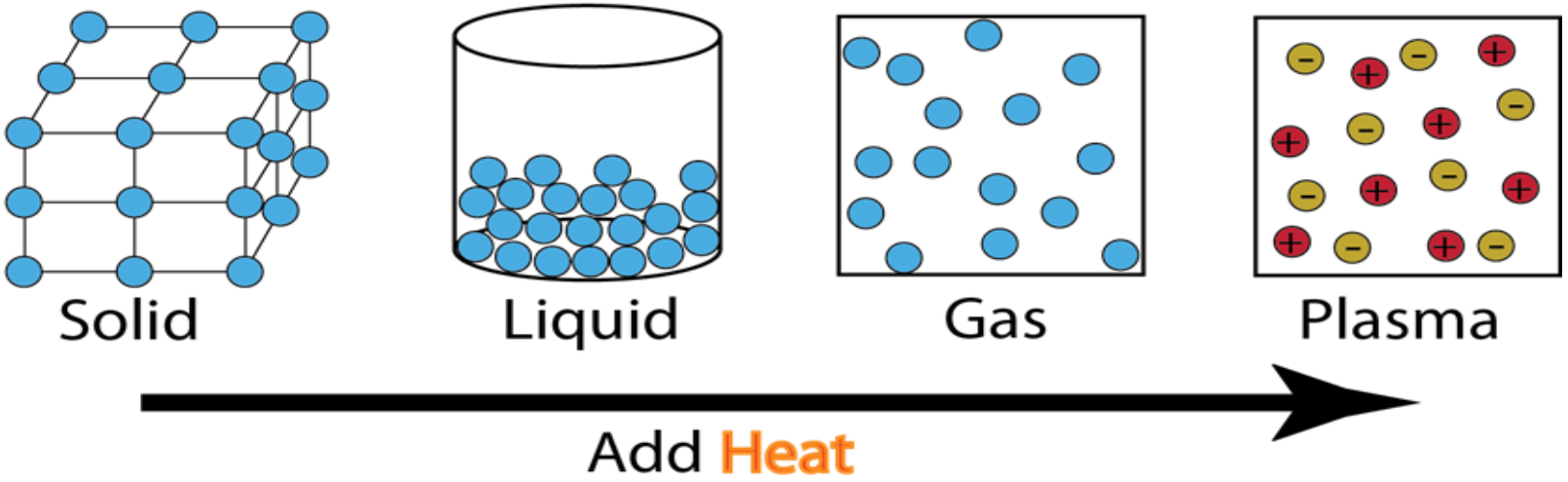
2) New direction in attoscience: Advancement of laser science and technology

Outline

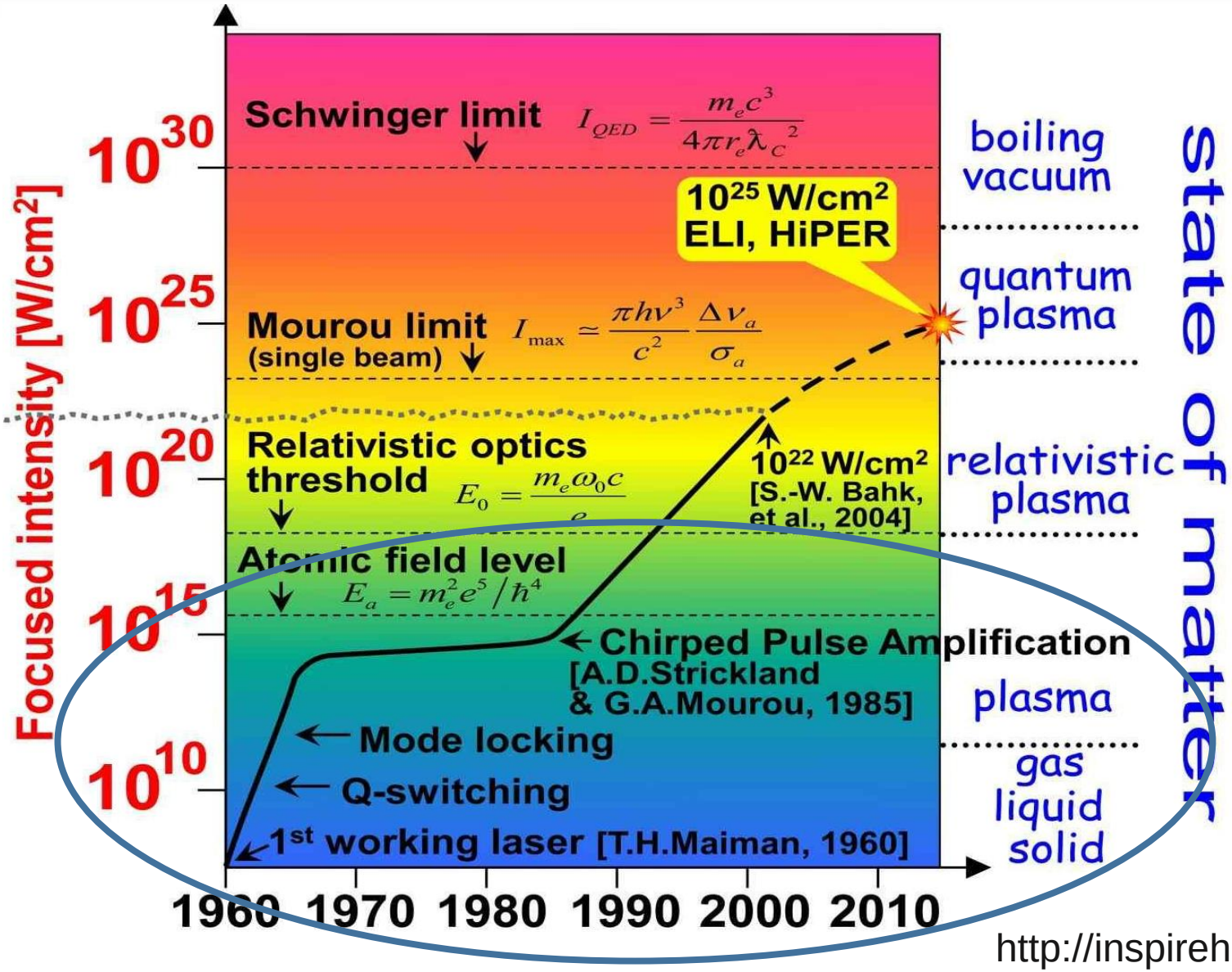
- Laser-matter interaction – different domains
- Tools to address the interaction
- Numerical simulations -using a common platform
- Adding results to repository- big data analysis.
- Some practical applications
  - ✓ Electronic structures of a material
  - ✓ Probing ultrafast processes in nanostructures

What happens when we shine a material with light



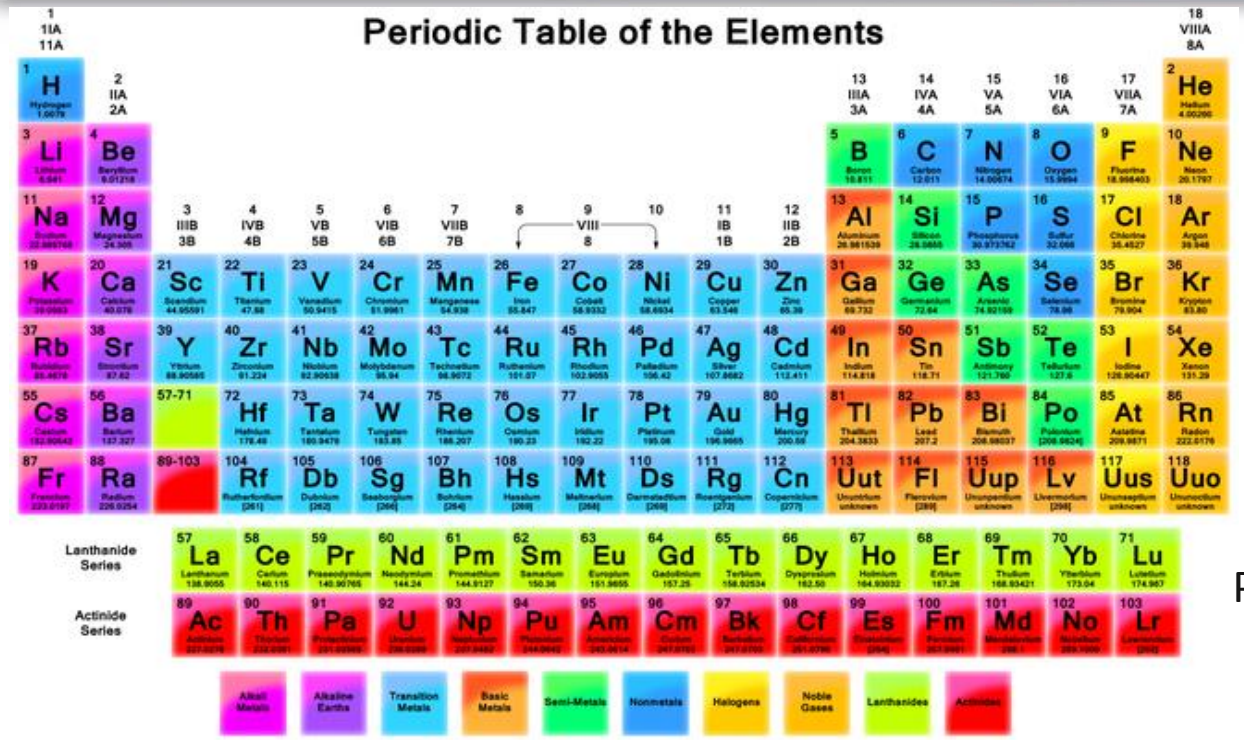


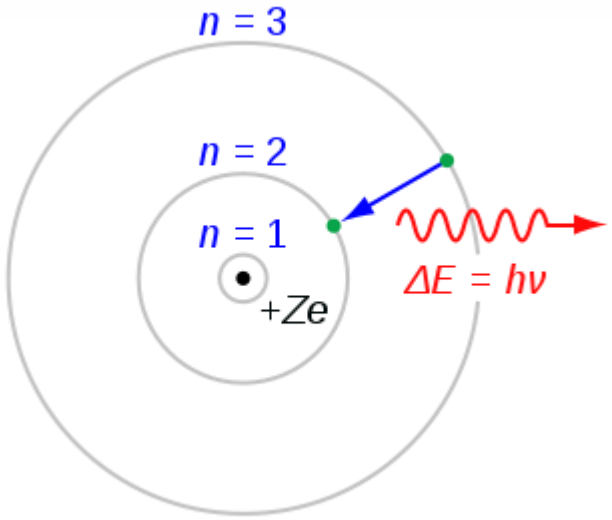
Which regime are we talking about?



http://inspirehep.net/

Use LASER to understand and control materials





Period of first Bohr orbit : 150 as

Control and trace the motion of atoms in molecules

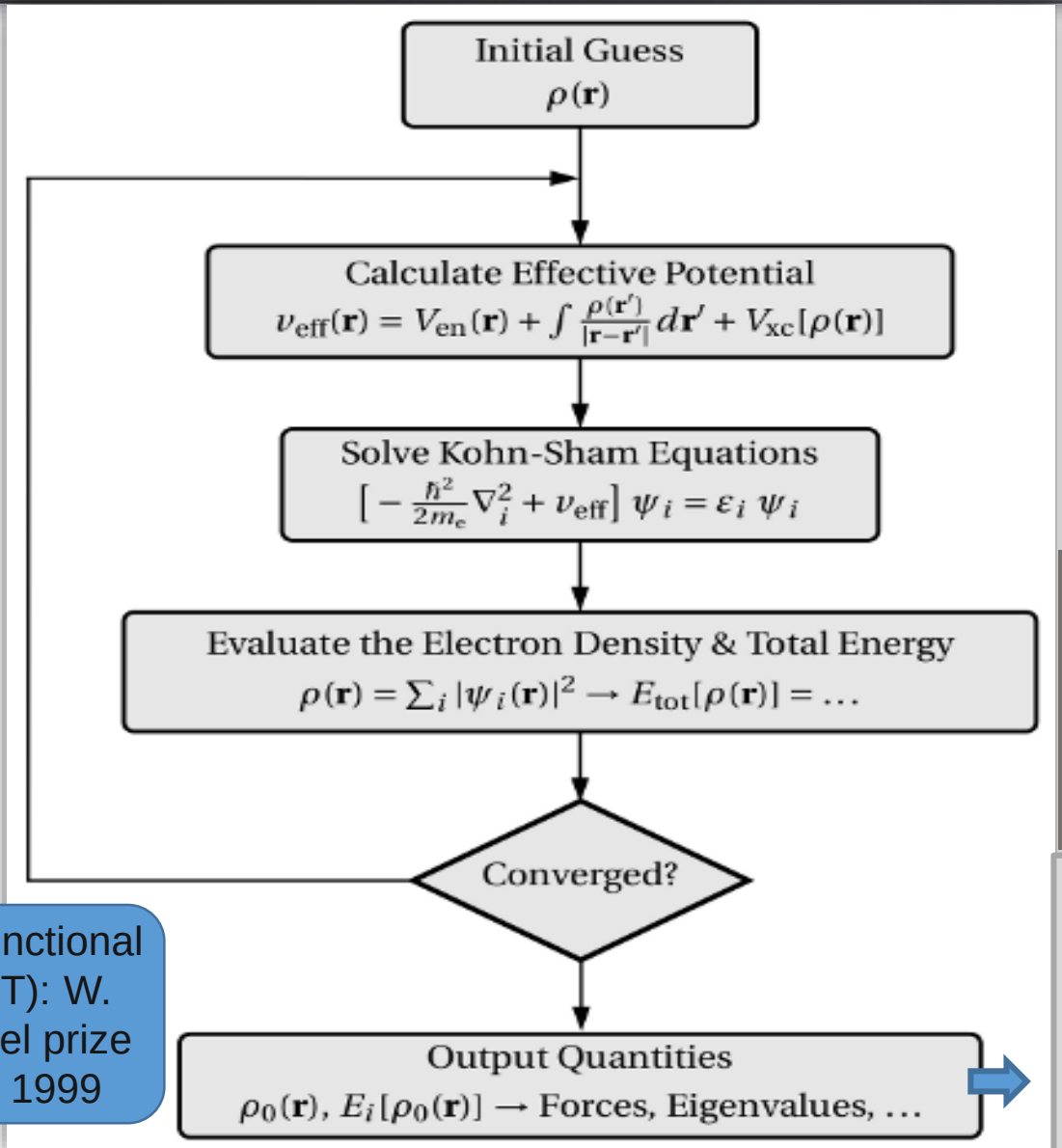
⇒ Control chemical reactions

Control & trace electrons inside atoms & molecules

Femto

Atto

How ab-initio method works?



- ✓ Quantum espresso (free)
- ✓ Octopus (free)
- ✓ VASP (licensed)
- ✓ Siesta (free)

TDDFT for excited state properties and dynamics.

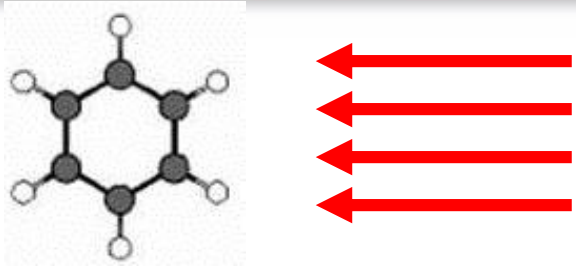
fundamental variable is the many-body charge density.

- ➢ Structure, energetics….
- ➢ Cheap, virtual experiment

Density Functional Theory(DFT): W. Kohn, Nobel prize Chemistry, 1999

Real-time electron dynamics in materials

Generic situation:
Molecule in laser field

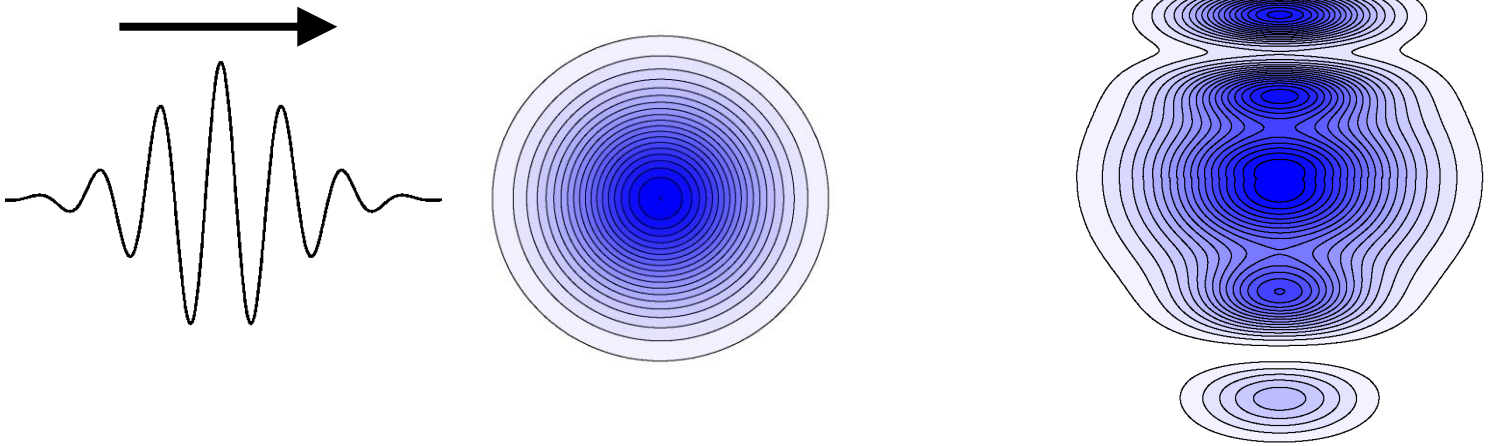


$$\hat{H}(t) = \hat{T}_e + \hat{W}_{ee} + \sum_{j,\alpha} - \frac{Z_\alpha e^2}{|r_j - R_\alpha|} + \vec{E} \cdot \vec{r}_j \cdot \sin \omega t$$

Strong laser ($v_{laser}(t) \geq v_{en}$) :

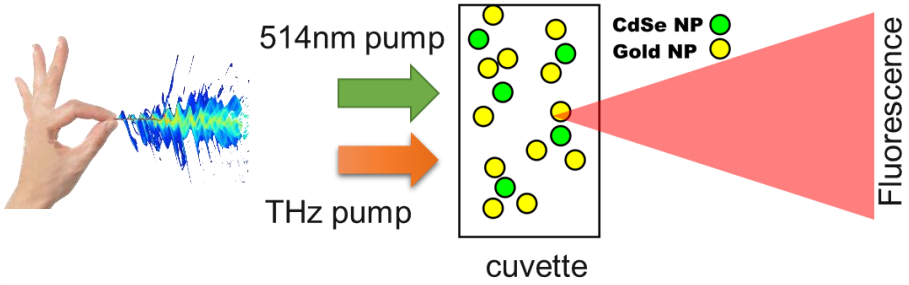
Non-perturbative solution of full TDSE required

Nonlinear response and ionization of atoms
and molecules in strong laser fields



THz spectroscopy lab - THz control in gas & solid phase

Exploring mechanism of terahertz generation from two-color laser induced air plasmas with high-resolution step scan FT VIS spectroscopy



Controlling vibrational, rotational, electronic populations from photodissociation processes with terahertz pulses

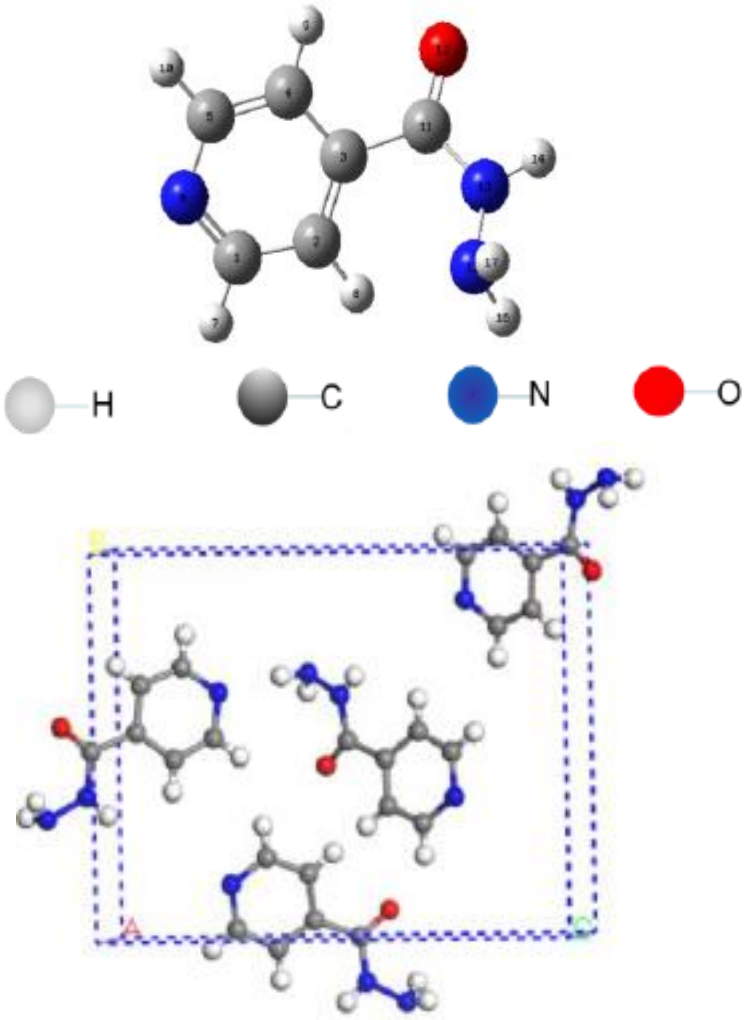
Example reaction…

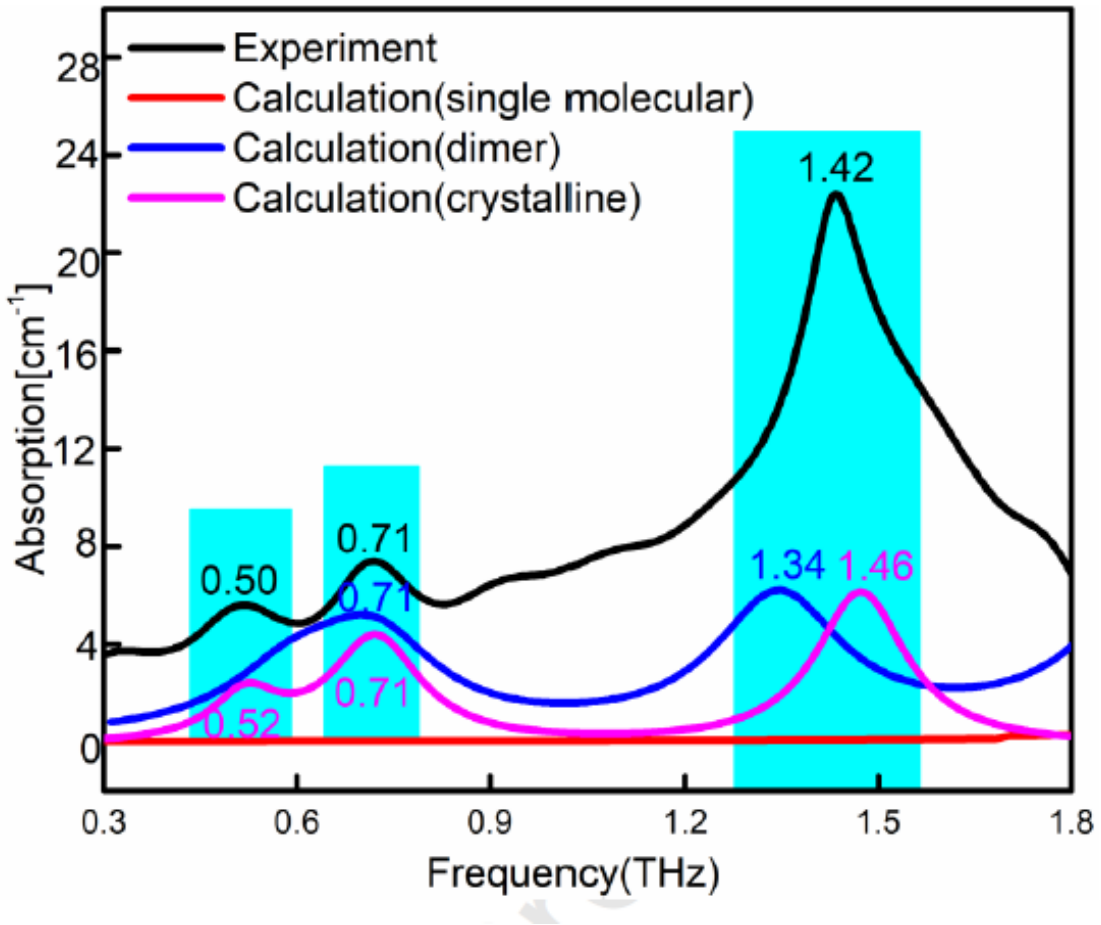
CHX_3+multiphoton(514nm)→CH(A)+Products

User experiment: Terahertz-driven Luminescence in CdSe Quantum Dots

THz spectroscopy + DFT….. Comprehensive approach

Isoniazid in molecular, and crystalline form…. Identifying suitable structures





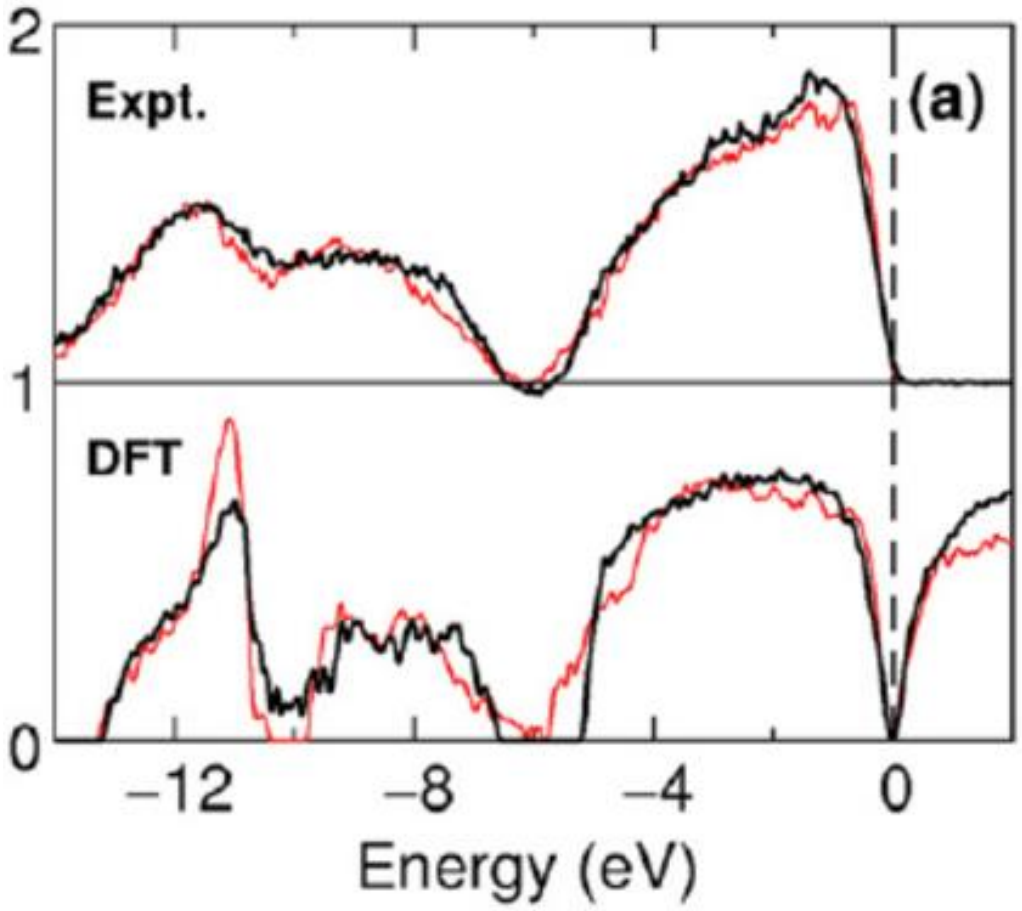
Crystalline structures lead to vibrational spectra closer to experiment

https://doi.org/10.1016/j.saa.2019.117591

DFT based tools: Virtual X—ray laboratory

Density functional study of amorphous, liquid and crystalline Ge 2Sb2Te5: Homopolar bonds and/or AB alternation?

J. Phys. Cond. Mat. 20(46):465103 (2008)

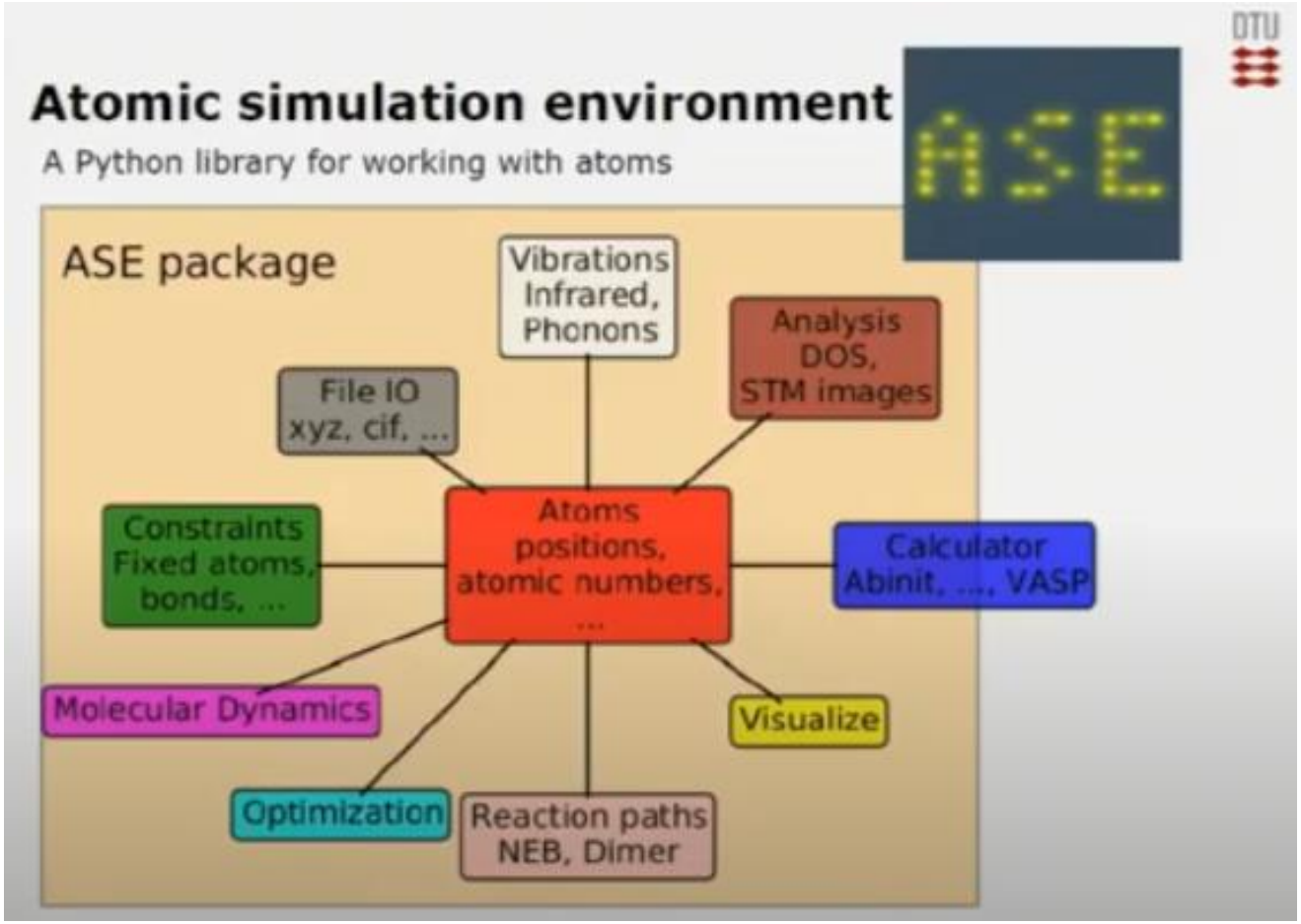


X-ray photoemission spectroscopy (XPS) valence band spectrum of a-(thick black) and c-GST (red/grey lines)

DOI: 10.1088/0953-8984/20/46/465103

A common ab-initio simulation platform… ASE

Atomistic simulation environment (ASE) for Density functional study



• Materials data & their structure

Level	Properties	Methods	Size
I	Atomic positions and nuclear charges, properties of free atoms, symmetry	Input: definition of material	10 kB - 10 MB
II			10 MB - 10 TB
III	optical spectra, electrical conductivity, phonon spectra, thermal conductivity, etc.	theory (MBPT),	1 GB - 1 TB
IV	Efficiency of solar cell, thermoelectric figu merit, turn-over frequency of catalyst, etc. as a function of temperature and pressure		10 kB - 1 MB

The amount of materials data produced on workstations, compute clusters, and supercomputers is growing exponentially.

Most of it is thrown away ….

• *No*vel *Ma*terials *D*iscovery (NOMAD)

- http://nomad-repository.eu

The ***NoMaD Repository***

Insight by sharing

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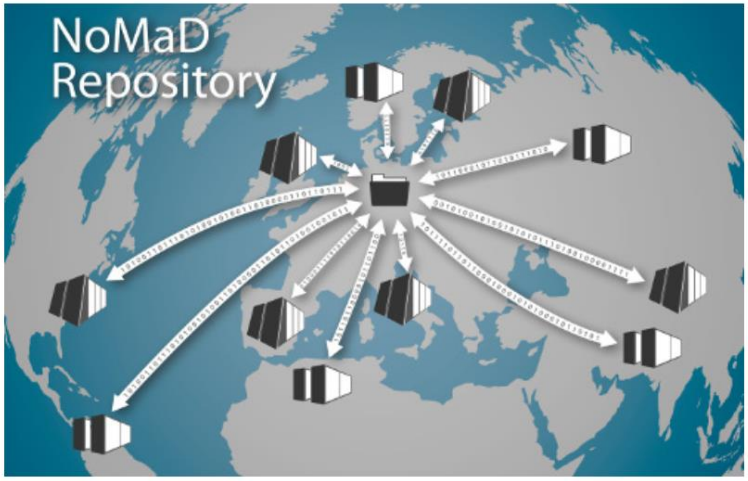
Welcome to the NoMaD Repository



The *NoMaD* (Novel Materials Discovery) *Repository* was established to host, organize, and share materials data.

NoMaD copes with the increasing demand and requirement of storing scientific data and making them available for longer periods. Rules of good scientific practice set by many funding agencies, worldwide, require keeping scientific data for 10 years. ***NoMaD*** offers this for free. ***NoMaD*** also facilitates research groups to share and exchange their results, inside a single group or between two or more, and to recall what was actually done some years ago.

The ***NoMaD Repository*** enables the confirmatory analysis of materials data, their reuse, and repurposing. Have a look at **youtube** to see our **movies on the concept and a basic tutorial.**

News

Currently, the NoMaD Repository contains

50,236,539

entries.

Upload to *NoMaD* from *MedeA* application ... more

Check for related **conferences and workshops**.

Financial Support

THANK YOU FOR YOUR ATTENTION!

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