



PaNOSC status update:

Mousumi Upadhyay Kahaly

Computational Materials Research, Theory & Simulation

ELI-ALPS, Szeged, Hungary

WP5 development sprint
20th to 30th April, 2020



European Union
European Regional
Development Fund



INVESTING IN YOUR FUTURE

The Research Institutes (sites) of ELI

ELI-DC Brussels

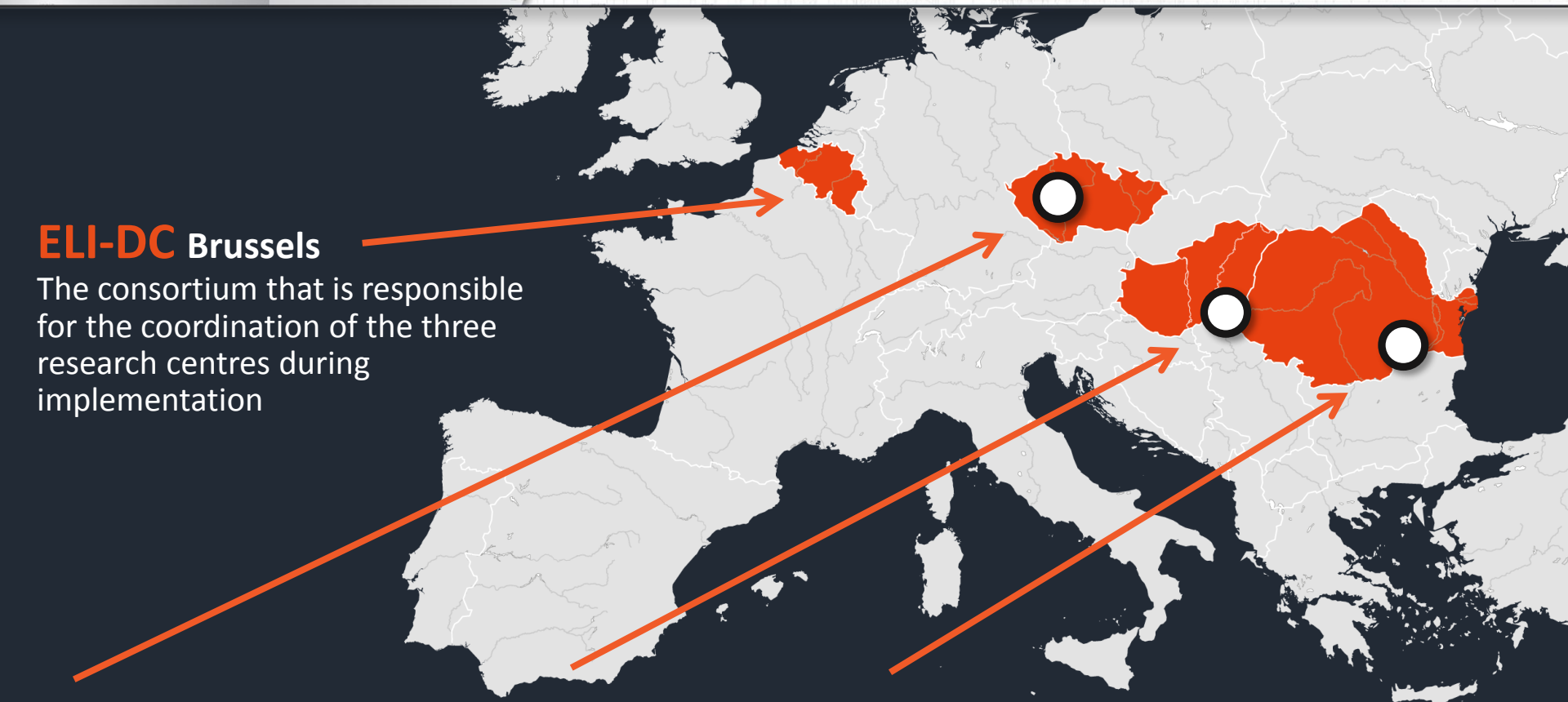
The consortium that is responsible for the coordination of the three research centres during implementation

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

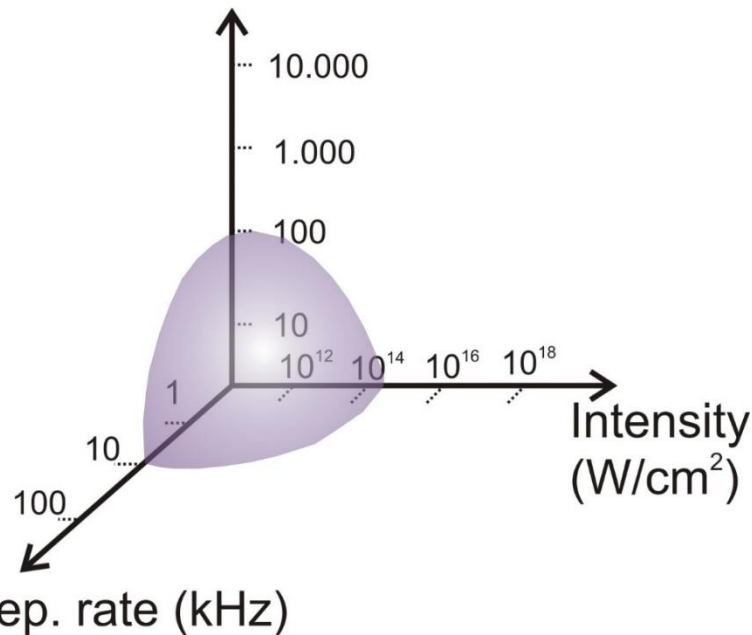
UHFS
Ultra-High-Field Science
unprecedented laser
field strength
(location: TBD)



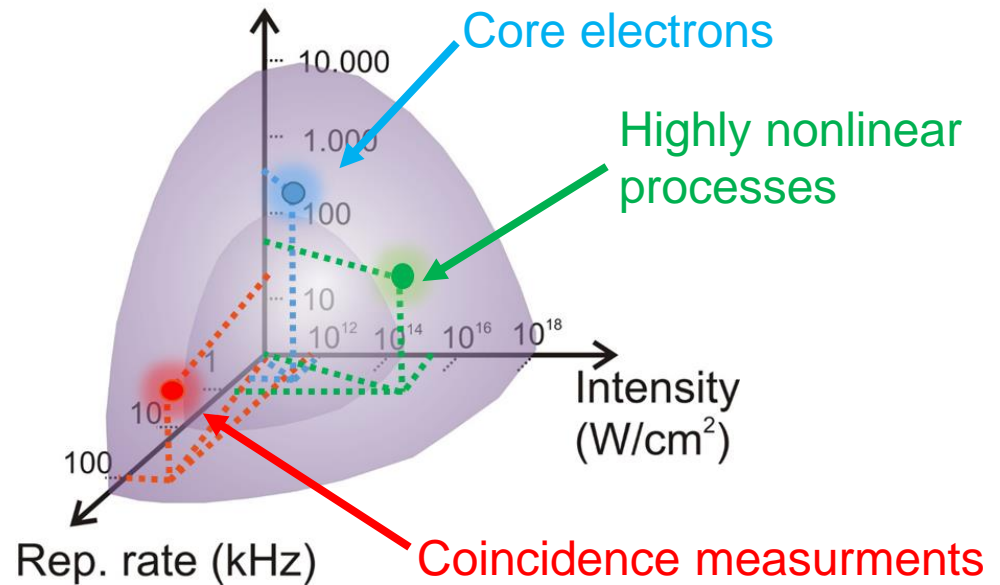
Activity range at ELI-ALPS

ELI-ALPS user facility

Photon energy (eV)



Photon energy (eV)



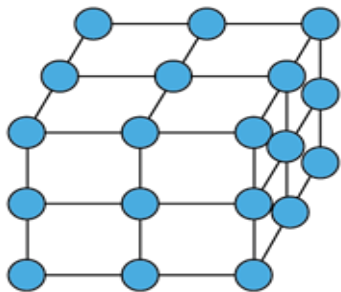
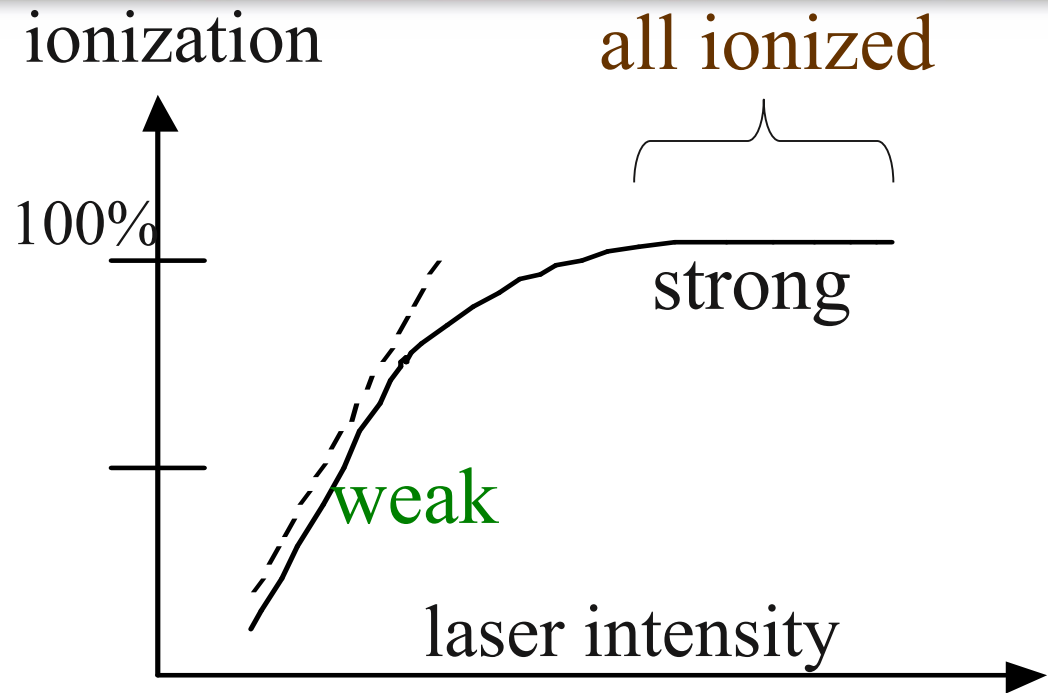
- 1) Generation of XUV/X-ray femto- and attosecond pulses
→ Attosecond scale of electron dynamics in atoms, molecules, plasmas and solids

ATTOSECOND Beamlines & User Facility

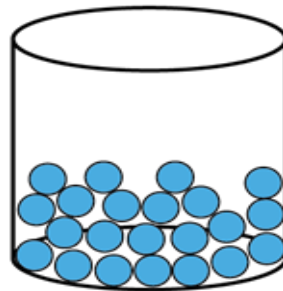
- 2) New direction in attoscience: Advancement of laser science and technology

- ❖ 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

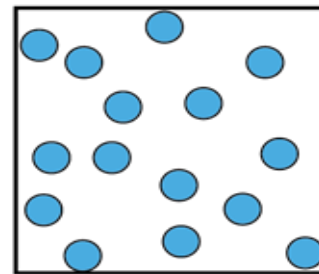
What happens when we shine a material with light



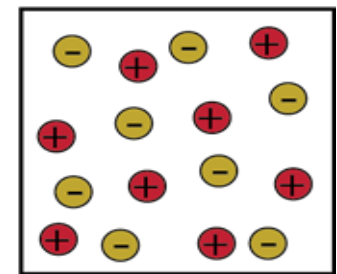
Solid



Liquid



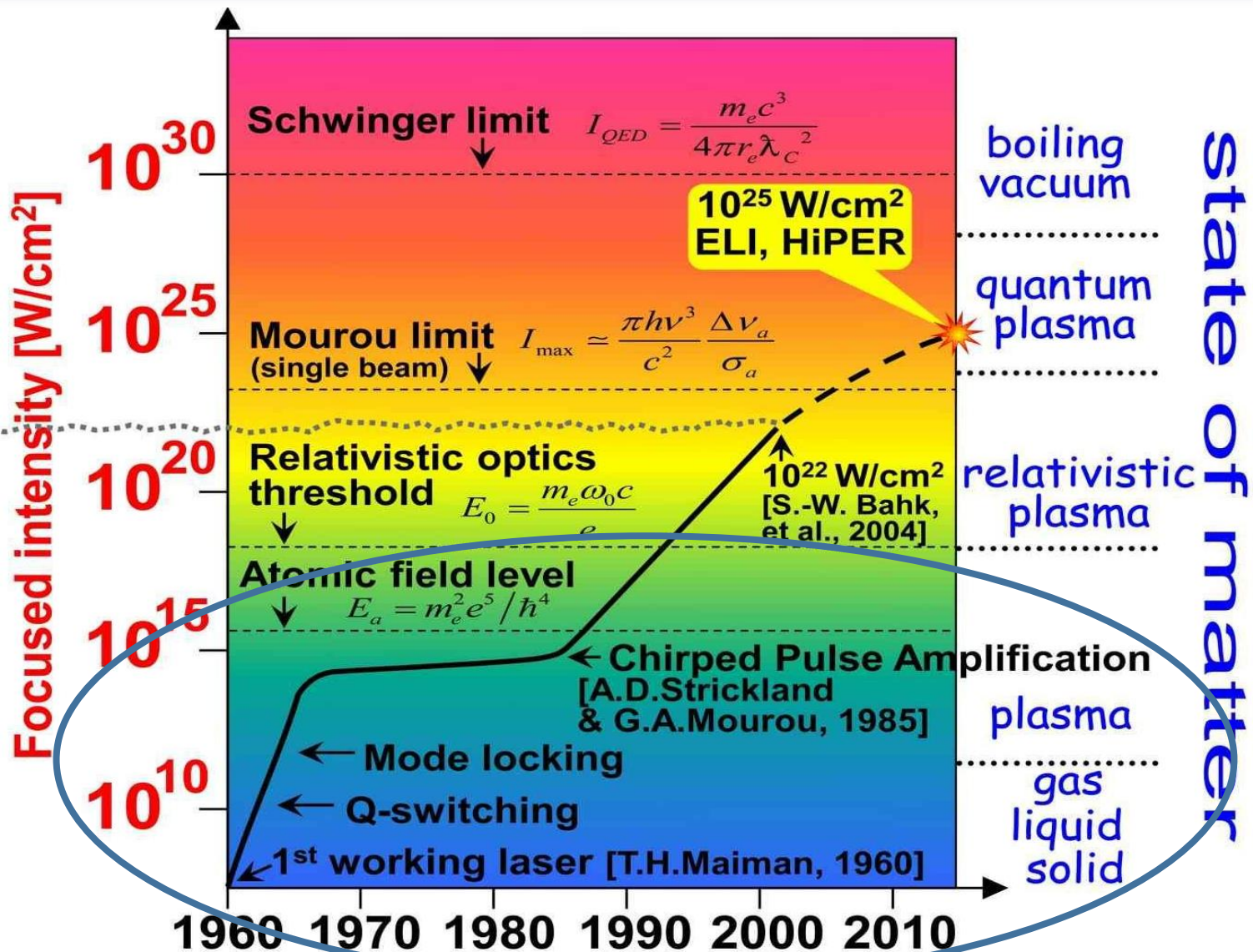
Gas



Plasma

Add Heat

Which regime are we talking about?



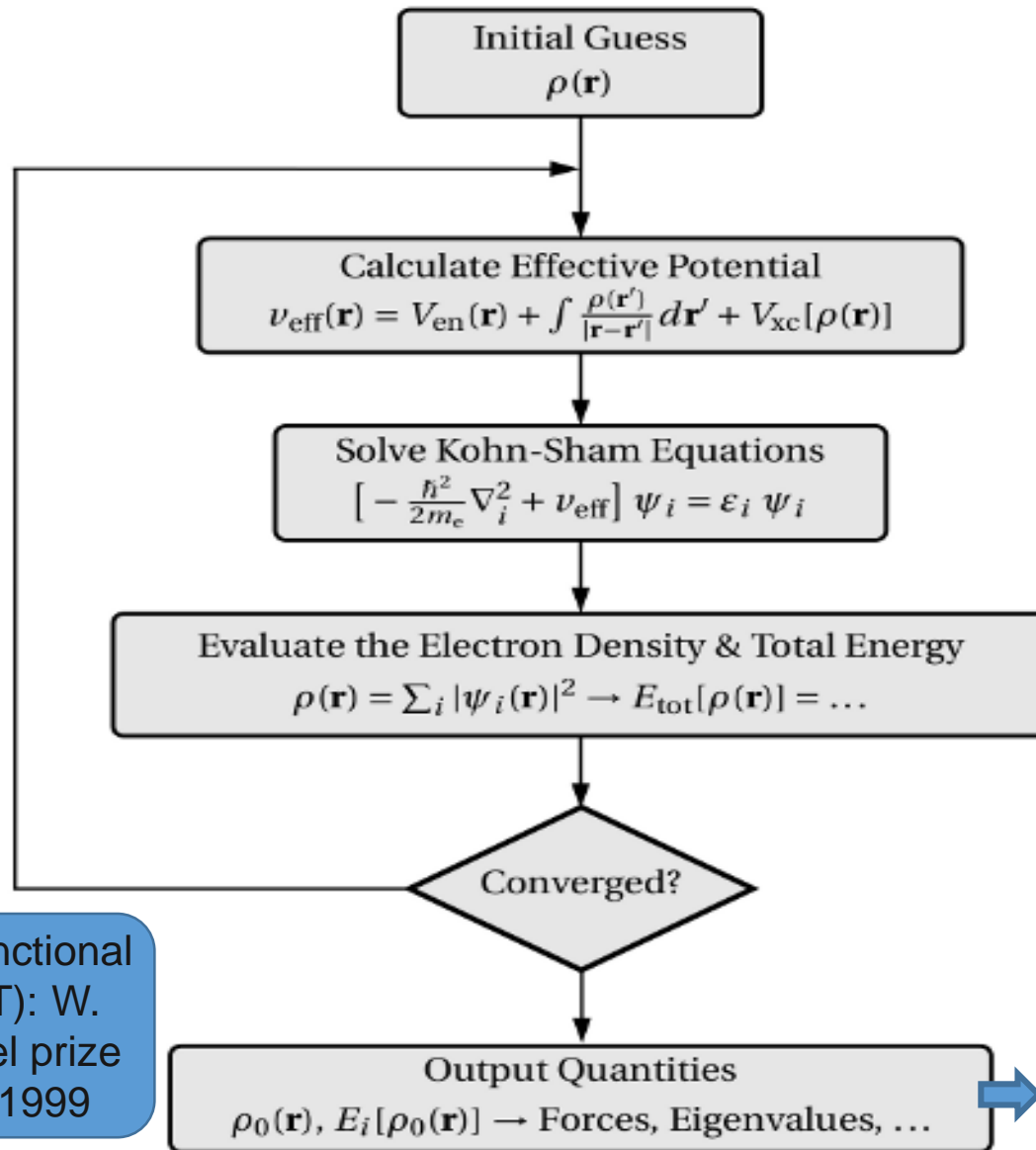
Use LASER to understand and control materials



Periodic Table of the Elements

Periodic Table of the Elements																			
1 H 1.00794												13 Al 26.981538	14 Si 28.0855	15 P 30.973762	16 S 32.06	17 Cl 35.4527	18 Ar 39.948		
2 He 4.002602																			
3 Li 6.941																			
4 Be 9.012182																			
5 B 10.811																			
6 C 12.011																			
7 N 14.00644																			
8 O 15.999																			
9 F 18.9984																			
10 Ne 20.1797																			
11 Na 22.989769																			
12 Mg 24.304																			
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16 S 32.06																			
17 Cl 35.4527																			
18 Ar 39.948																			
19 K 39.0983																			
20 Ca 40.078																			
21 Sc 44.95591																			
22 Ti 47.88																			
23 V 50.9415																			
24 Cr 51.9961																			
25 Mn 54.938																			
26 Fe 55.847																			
27 Co 58.9332																			
28 Ni 58.6934																			
29 Cu 63.546																			
30 Zn 65.39																			
31 Ga 69.723																			
32 Ge 72.64																			
33 As 74.921595																			
34 Se 78.96																			
35 Br 79.904																			
36 Kr 83.80																			
37 Rb 85.4678																			
38 Sr 87.62																			
39 Y 88.90585																			
40 Zr 91.224																			
41 Nb 92.90638																			
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45 Rh 102.9055																			
46 Pd 106.42																			
47 Ag 107.8662																			
48 Cd 112.411																			
49 In 114.818																			
50 Sn 118.71																			
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52 Te 127.6																			
53 I 126.90447																			
54 Xe 131.29																			
55 Cs 132.90545																			
56 Ba 137.327																			
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73 Ta 180.9479																			
74 W 183.85																			
75 Re 186.207																			
76 Os 190.23																			
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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....

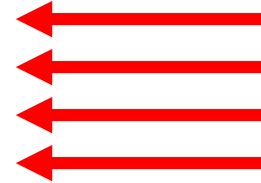
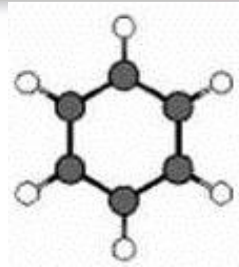
➤ Cheap, virtual experiment

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

Real-time electron dynamics in materials



Generic situation: Molecule in laser field

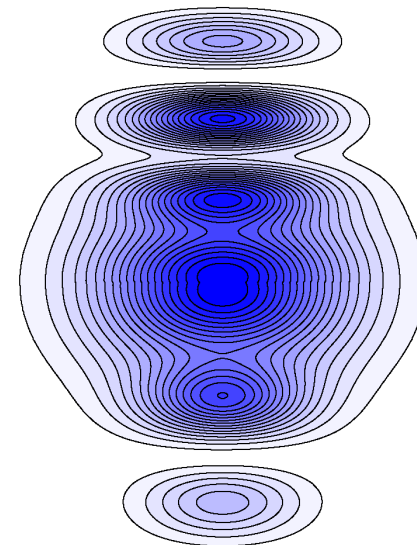
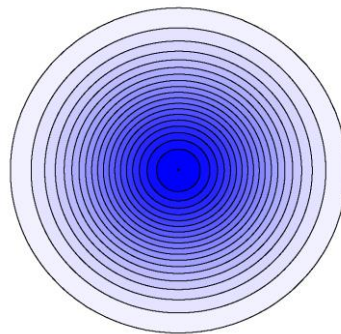
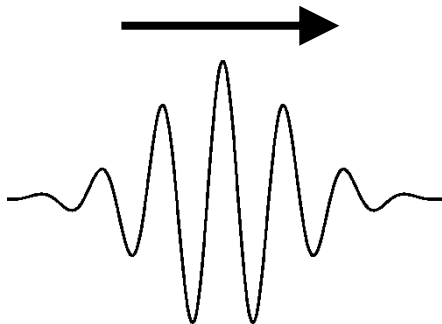


$$\hat{H}(\mathbf{t}) = \hat{T}_e + \hat{W}_{ee} + \sum_{j,\alpha} - \frac{Z_\alpha e^2}{|\mathbf{r}_j - \mathbf{R}_\alpha|} + \vec{E} \cdot \vec{r}_j \cdot \sin \omega t$$

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

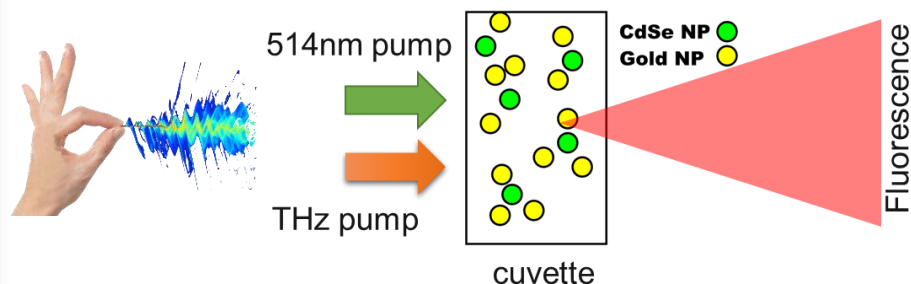
Non-perturbative solution of full TDSE required

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





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...

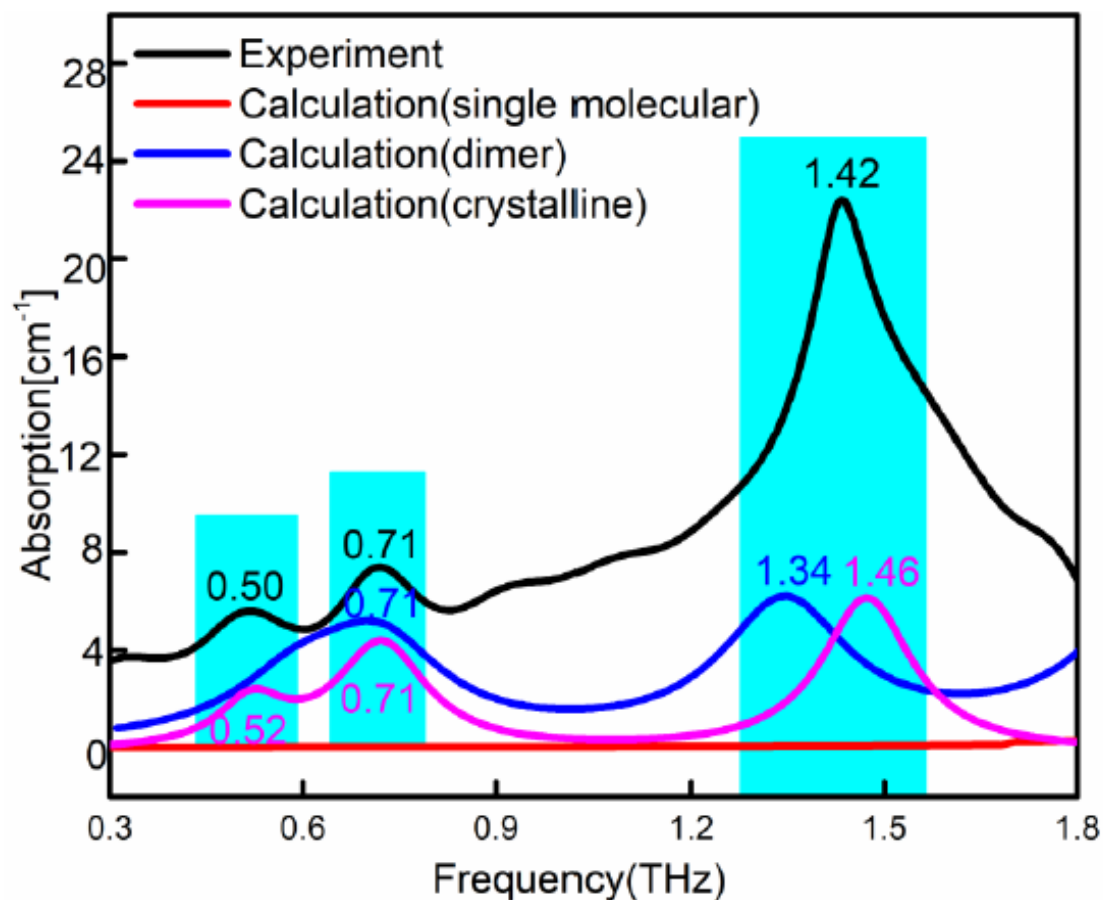
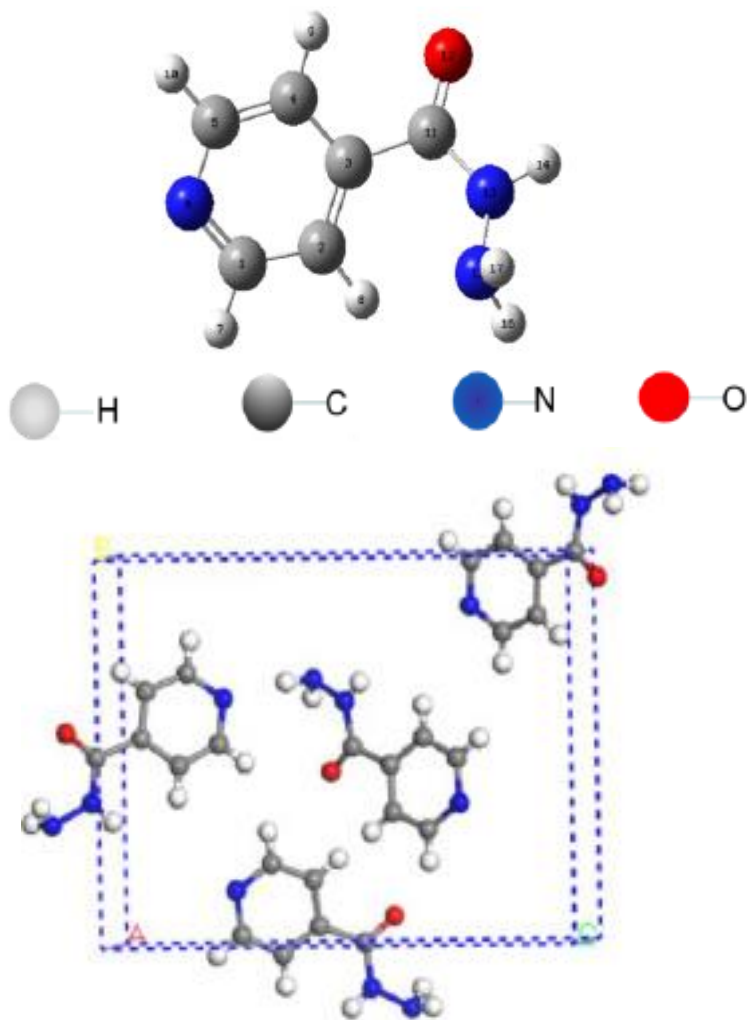


User experiment: Terahertz-driven Luminescence in CdSe Quantum Dots

THz spectroscopy + DFT..... Comprehensive approach



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



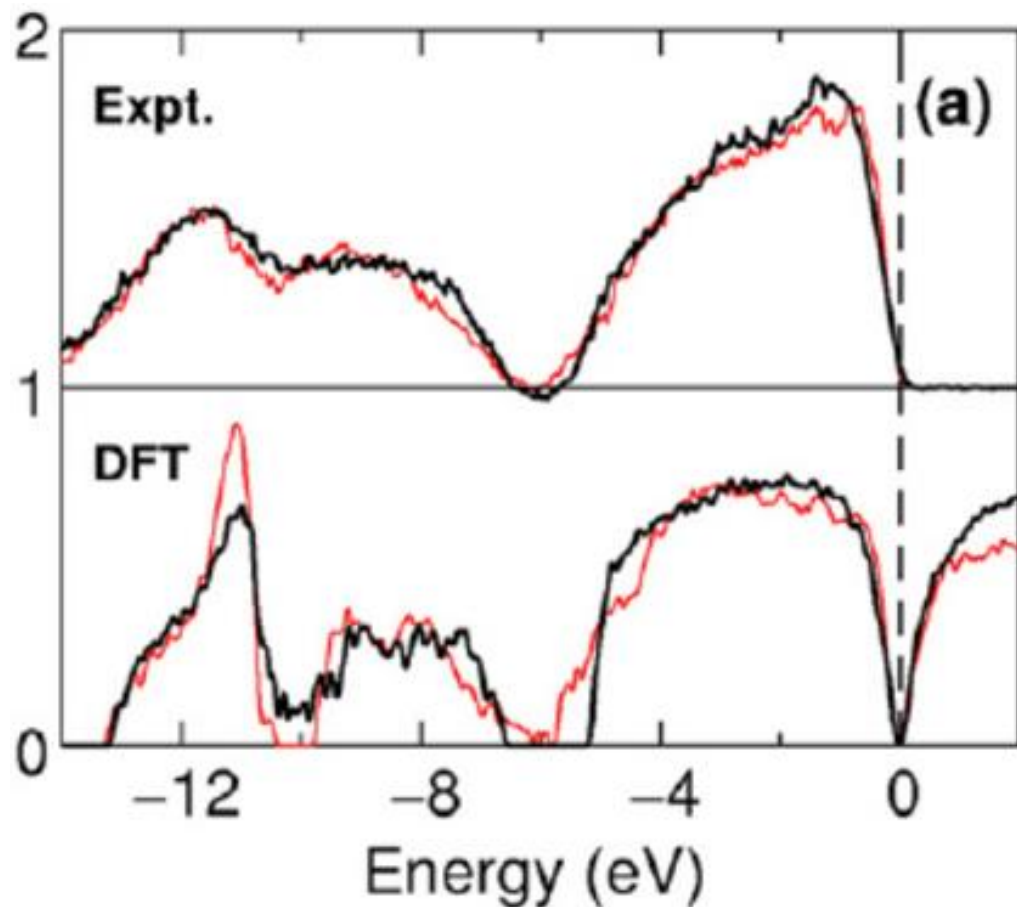
Crystalline structures lead to vibrational spectra closer to experiment

DFT based tools: Virtual X—ray laboratory



Density functional study of amorphous, liquid and crystalline Ge₂Sb₂Te₅:
Homopolar bonds and/or AB alternation?

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

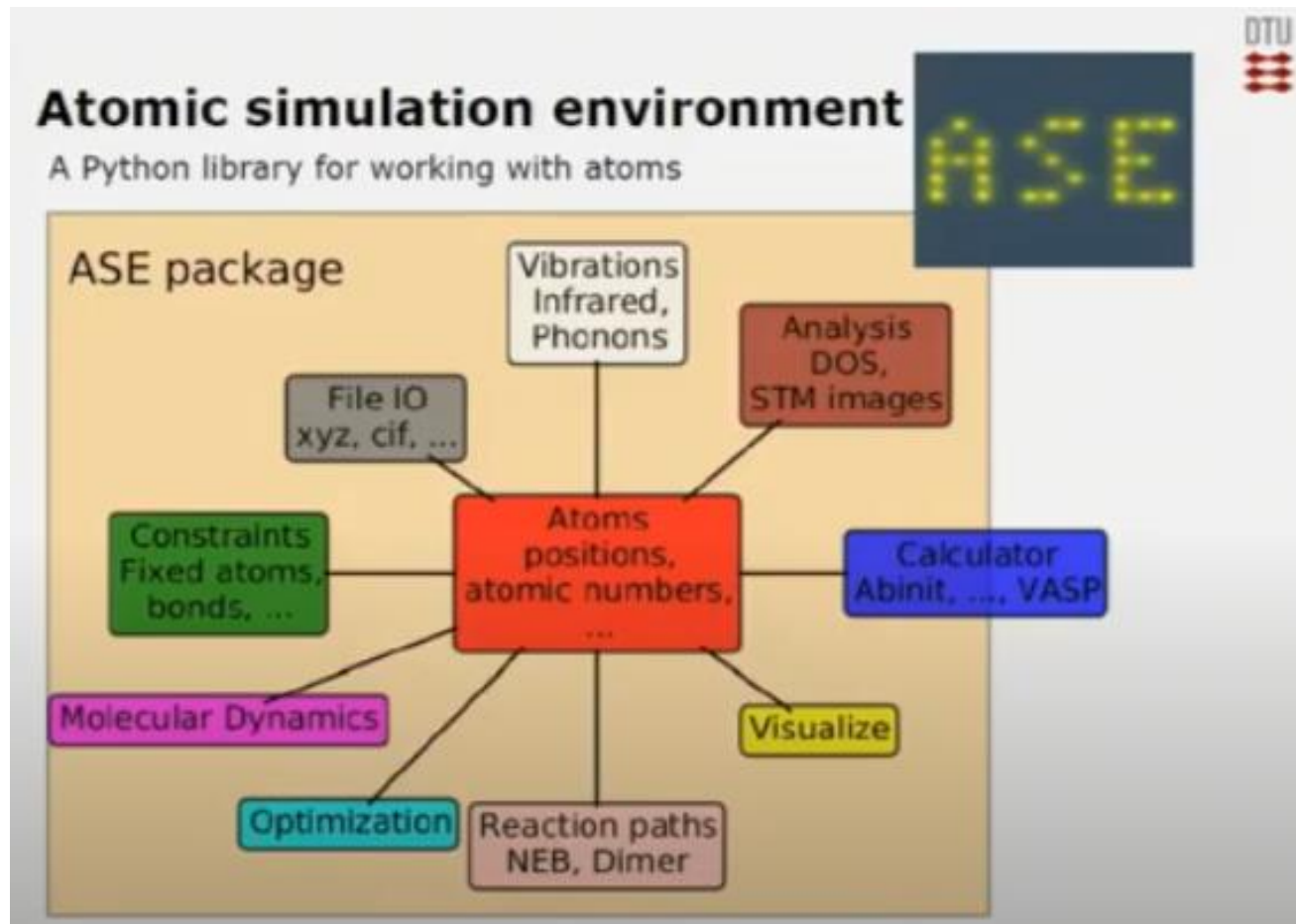


X-ray photoemission
spectroscopy (XPS) valence
band spectrum of a-(thick
black) and c-GST (red/grey
lines)

A common ab-initio simulation platform... ASE


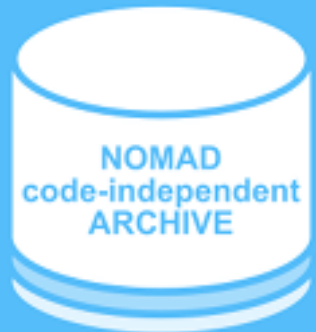


Atomistic simulation environment (ASE) for Density functional study



• Materials data & their structure

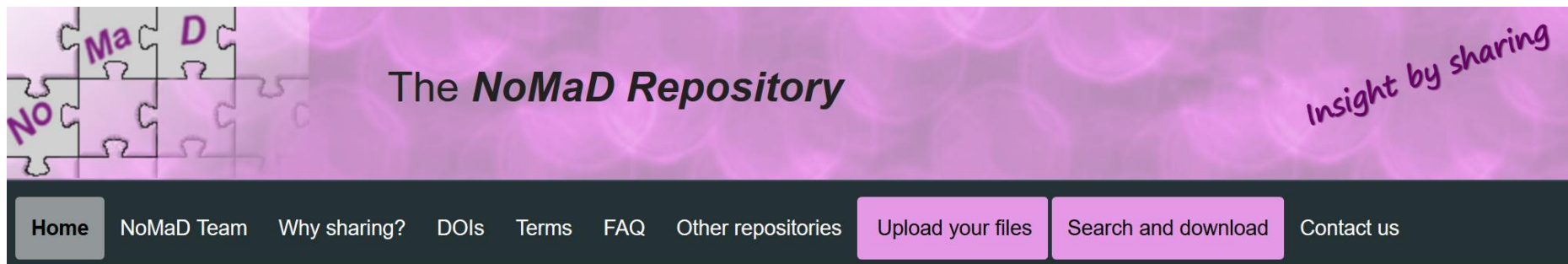


Level	Properties	Methods	Size
I	Atomic positions and nuclear charges, properties of free atoms, symmetry	Input: definition of material	10 kB - 10 MB
II	<p>The amount of materials data produced on workstations, compute clusters, and supercomputers is growing exponentially. Most of it is thrown away</p>		10 MB - 10 TB
III			1 GB - 1 TB
IV	Efficiency of solar cell, thermoelectric figure of merit, turn-over frequency of catalyst, etc. as a function of temperature and pressure	 	10 kB - 1 MB

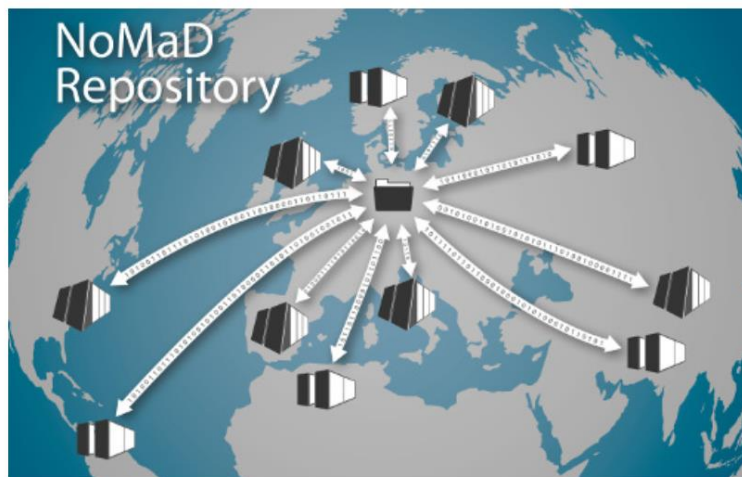
- **Novel Materials Discovery (NOMAD)**



- <http://nomad-repository.eu>



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.

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](#)

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**.

THANK YOU FOR YOUR ATTENTION!

SZÉCHENYI 2020



HUNGARIAN
GOVERNMENT

European Union
European Regional
Development Fund



INVESTING IN YOUR FUTURE