

# OPEN MOLECULAR SCIENCES FOR RENEWABLE ENERGIES

On the role of shareable (re-usable) molecular knowledge in supporting innovation: the exploitation of renewable energies

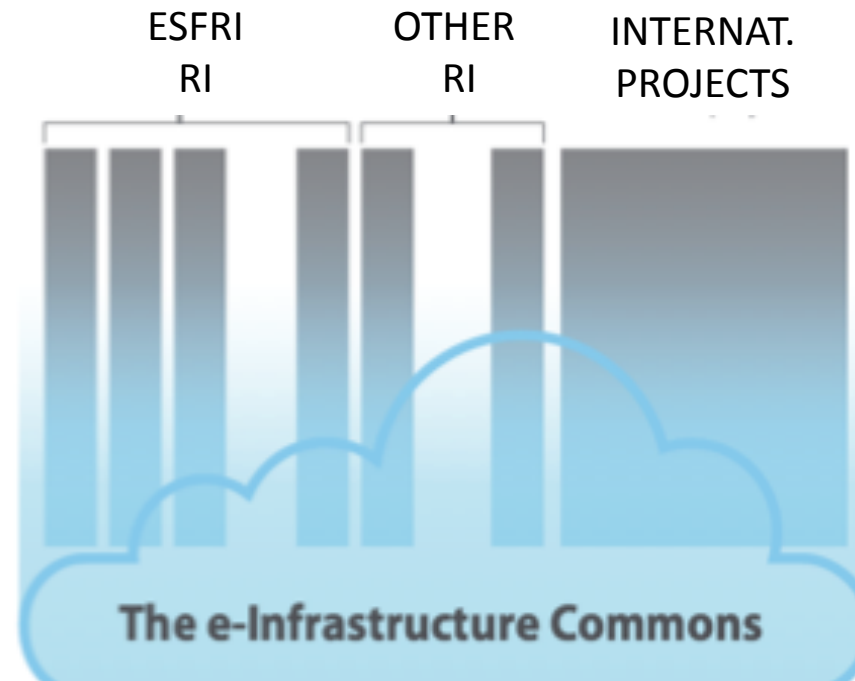
*Antonio Laganà*

Department of Chemistry, Biology and Biotechnologies,  
University of Perugia, IT

# THE NEED FOR OPEN SCIENCE

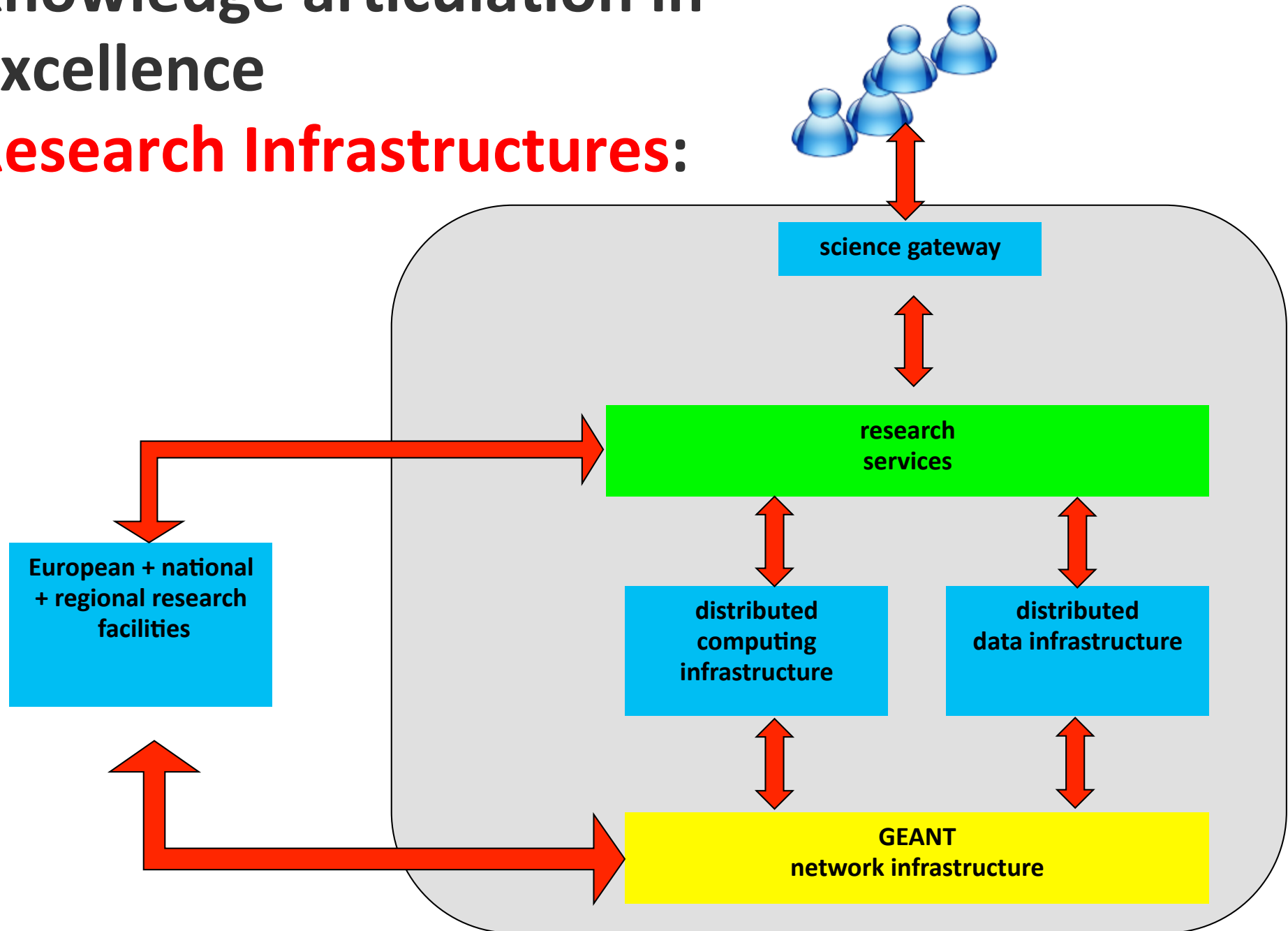
- In research and society OPEN SCIENCE (free and full accessibility of scientific achievements) is **the key enabling factor for progress** because it:
  - changes the modus operandi of research by opening new possibilities for **geographically distributed collaboration and knowledge sharing**
  - fosters **data reuse and data-driven science** with (larger) open access to information and scientific results transforming how science is made

ESFRI  
EUROPEAN STRATEGY FORUM

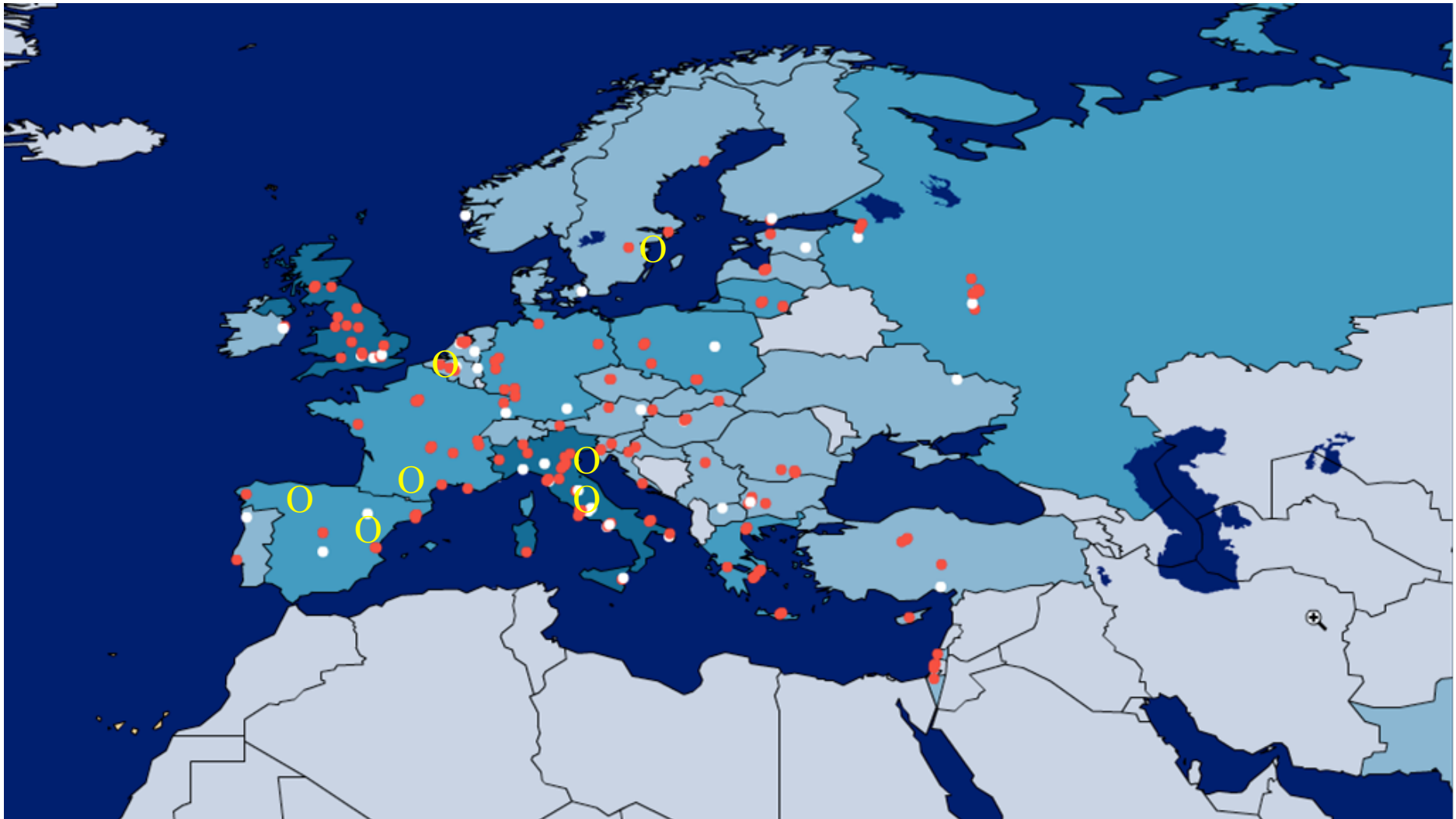


# Knowledge articulation in excellence

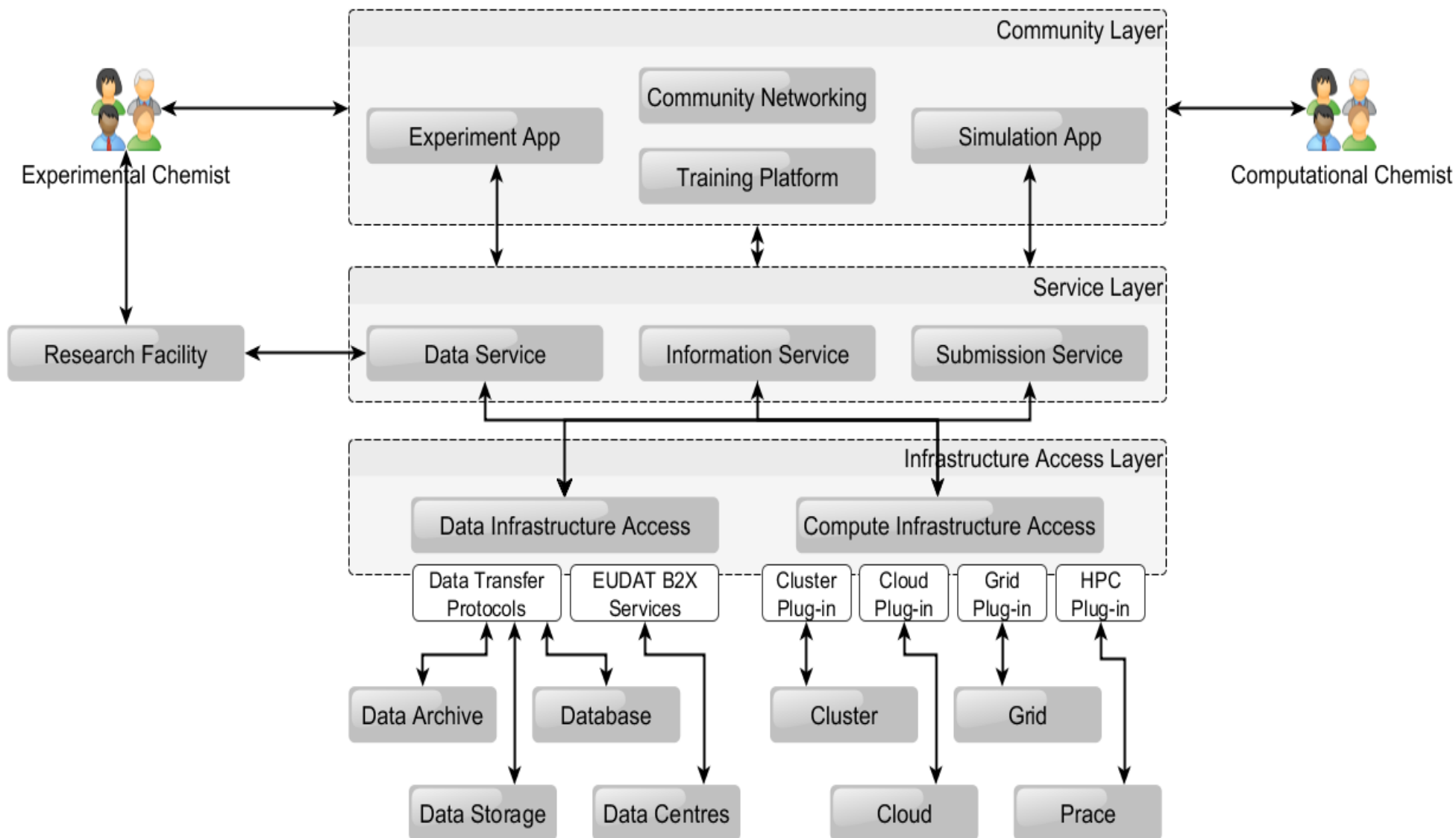
## Research Infrastructures:



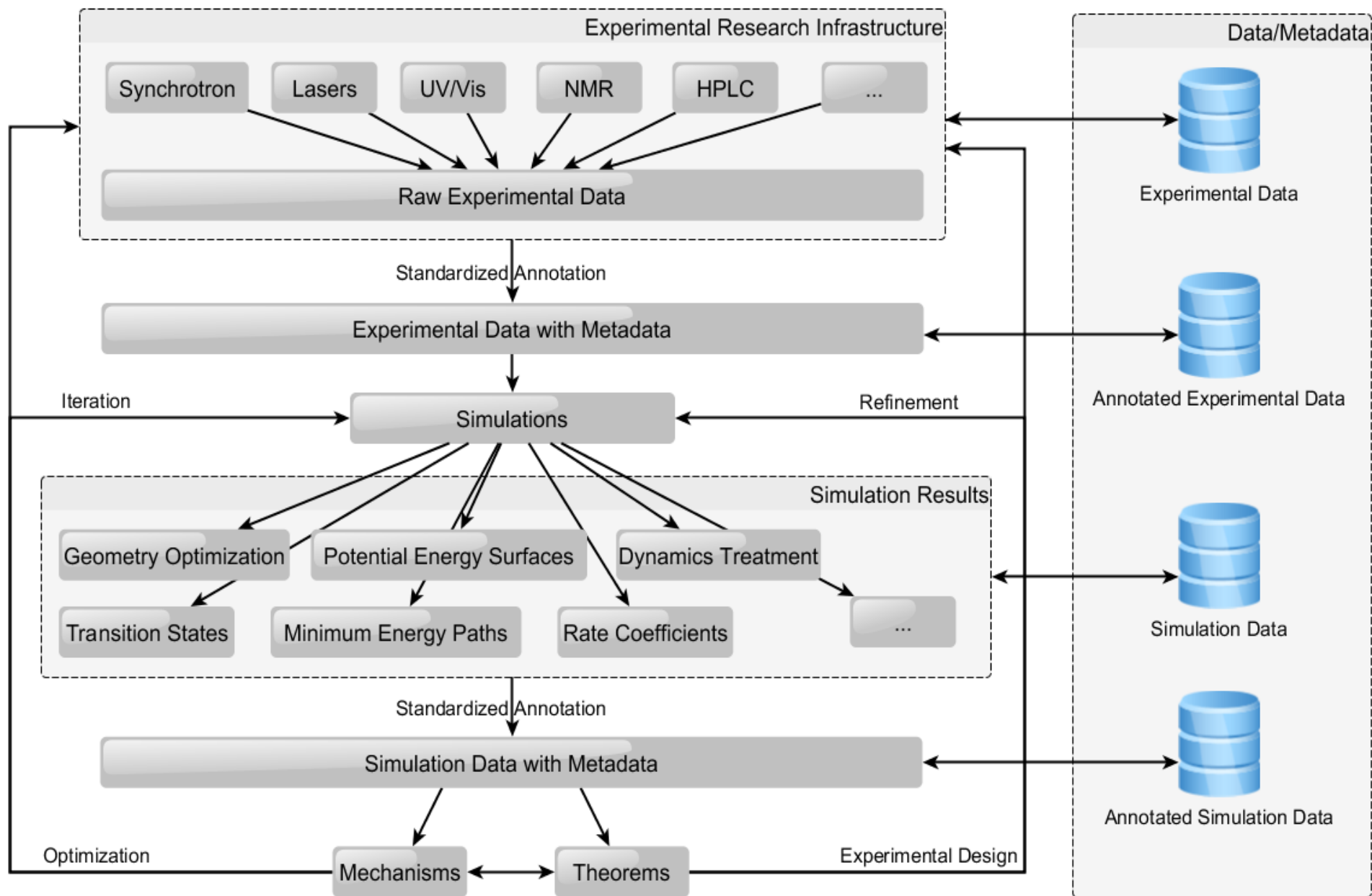
- EUROPEAN GRID INFRASTRUCTURE PRODUCTION GRID
- NETWORK OF THE FRE-Methane PROPOSAL



# NETWORKING THEORY and EXPERIMENT

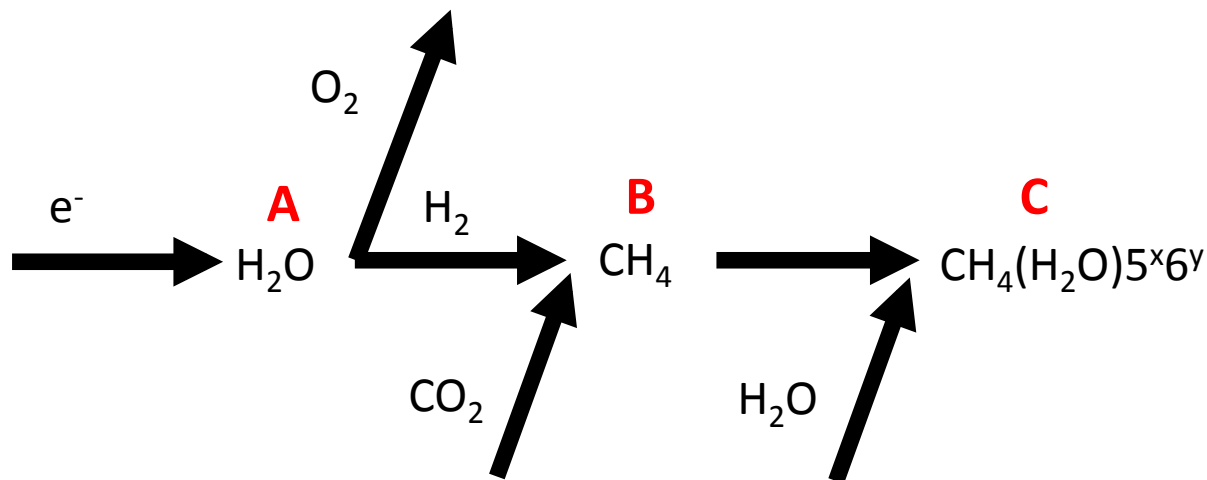


# MOLECULAR THEORY AND EXPERIMENT

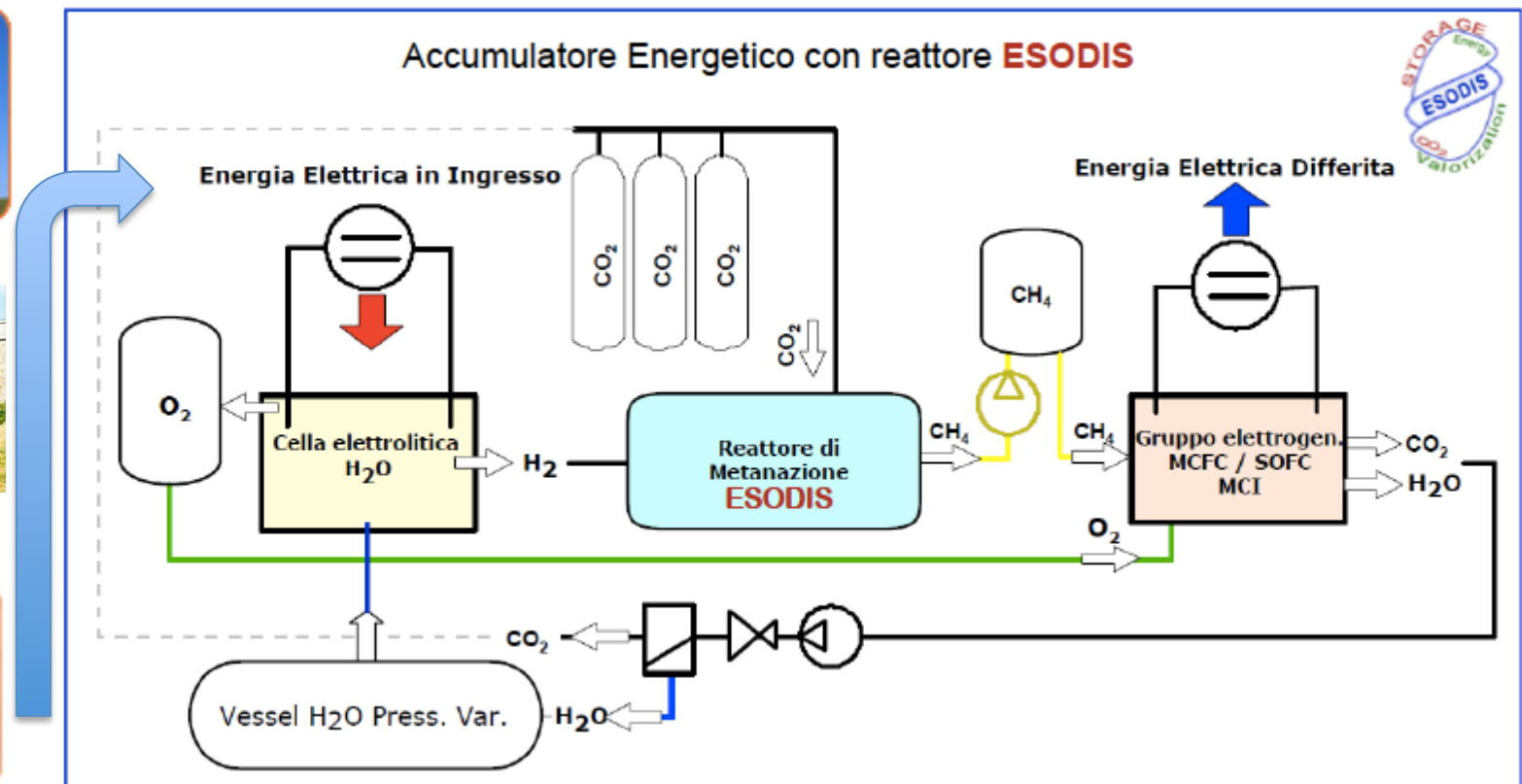


# THE OVERALL SCHEME OF THE FREE-METHANE PROPOSAL

- A) an innovative electrolyser producing  $H_2$  with an increase of the yield/cost ratio 300% larger than that of basic versions of commercial electrolysers,
- B) a new heterogeneous/homogeneous catalytic reactor of 50 kW using  $CO_2$  to produce synthetic fuel (mainly methane)
- C) a methane clathrate hydrate formation reactor for storing methane (a technology 400% cheaper than the traditional cooling and compressing for bottling) for its deferred use



# OUR CASE STUDY: RENEWABLE ENERGIES AND CARBON NEUTRAL FUELS





# SOCIETAL ACHIEVEMENTS

- MATCH large demand of carbon neutral fuels
- RE-USE CO<sub>2</sub>
- STORE renewable energy for deferred use.

# TECHNOLOGICAL INNOVATION

- NOVEL electrolyser of water
- EFFICIENT methanator of CO<sub>2</sub> (solid state cathalysis or gas phase process)
- SAFE and cheap transportantion
- **laboratory validation (TLR 4).**

# THE PARTNERS for an H2020 PROPOSAL

Acronym	Participant organisation name
UNIPG	University of Perugia
UB	University of Barcelona
LCPQ	University of Toulouse
ENEA	ENEA ( <u>Agenzia Nazionale per le Nuove Technologie, L'Energia e lo Sviluppo Economico Sostenibile</u> )
EHU	Universidad del <u>Pais Vasco/Euskal Herriko Unibertsitatea</u>
RPC	RPC <u>srl</u>
MUP	Master-up <u>s.r.l.</u>
BCO	<u>Blurock Consulting AB</u>
ECTN	European Chemistry Thematic Network Association

# COMPETENCE LINES

- Chemical dynamics, kinetics and homo- and heterogeneous catalysis and energetics for renewable energy storage as chemicals. (EHU, UB, UNIPG, ENEA, LCPCQ, RPC)
- KNOWLEDGE Handling (ENEA, MUP, ECTN, BCO)

# DYNAMICS AND KINETICS OF THE SABATIER REACTION

Kinetic Monte Carlo (KMC):

- State-to-state method (trajectory independent)
- Acquire the list of feasible pathway steps
- Initial reaction conditions ( $p$ ,  $T$ ,  $x_i$ )
- Lattice type to define neighbours

# Kinetic Monte Carlo features

- Transition probabilities obtained from rate coefficients ( $r_{ij}$ )
- Rate coefficients are computed using Transition State Theory
- Energy barriers are taken from bibliography<sup>[1-3]</sup>
- A variable timestep is adopted:

$$\Delta t = \frac{1}{\sum r_{ij}}$$

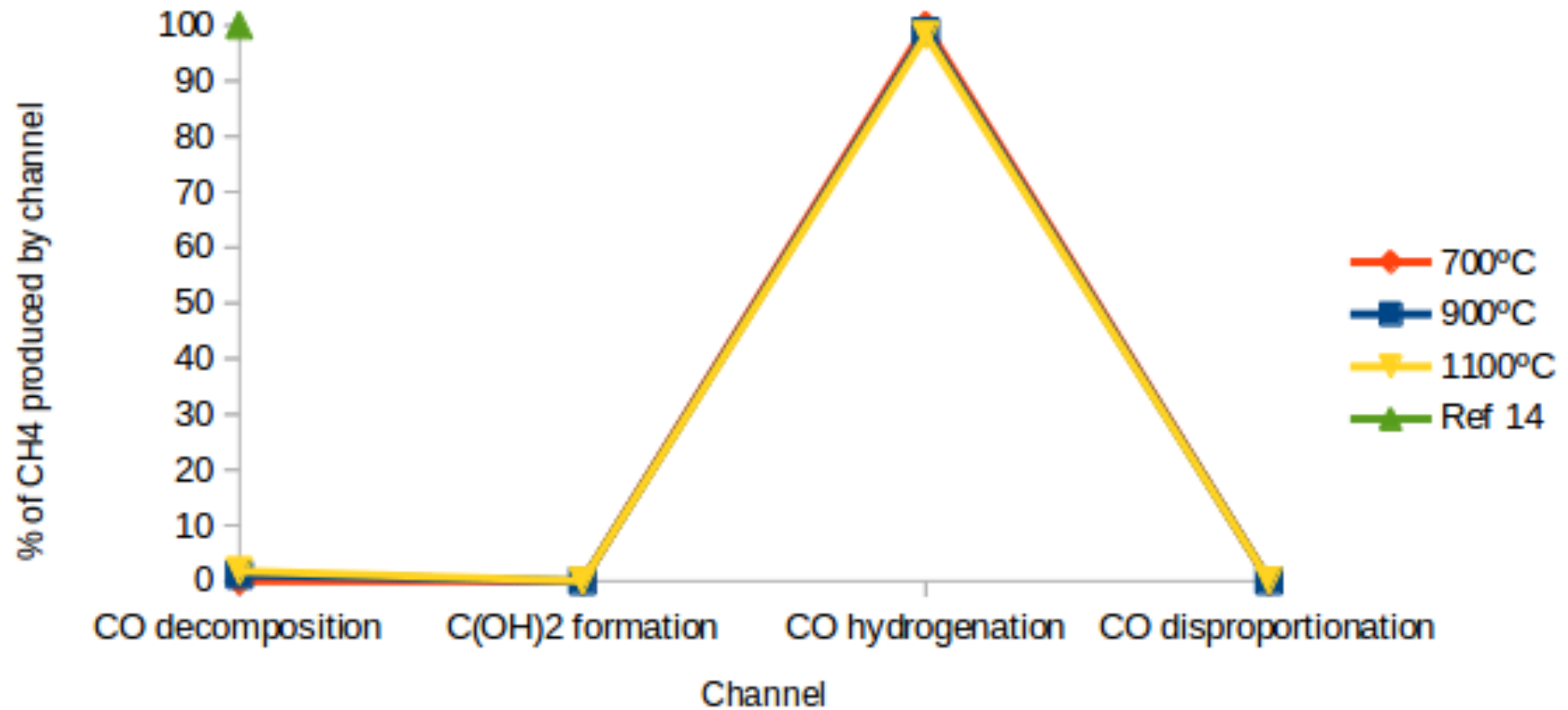
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- <sup>1</sup>Blaylock et al. J. Phys. Chem. C, Vol. 113, No. 12, 2009, 4898–4908.
  - <sup>2</sup>J. Ren et al. Applied Surface Science 351 (2015) 504–516.
  - <sup>3</sup>Catapan et al J. Phys. Chem. C 2012, 116, 20281–20291.

# List of elementary steps

	Energy Barriers (kJ/mol)			
	Used		Other data from Bibliography	
	Forward	Reverse <sup>a</sup>	Forward	Reverse
$\text{CO}_2 + * \leftrightarrow \text{CO}_2^*$	0 <sup>[8]</sup>	8.3 <sup>[9]</sup>		27.3 <sup>[11]</sup>
$\text{H}_2 + 2* \leftrightarrow 2\text{H}^*$	4 <sup>[8]</sup>	77.1 <sup>[9]</sup>	7.7 <sup>[10]</sup>	95.0 <sup>[12]</sup> , 132.2 <sup>[10]</sup>
$\text{CO} + * \leftrightarrow \text{CO}^*$	0 <sup>[8]</sup>	127.7 <sup>[9]</sup>		115 <sup>[12]</sup>
$\text{H}_2\text{O} + * \leftrightarrow \text{H}_2\text{O}^*$	0 <sup>[8]</sup>	49.0 <sup>[9]</sup>		64.4 <sup>[12]</sup>
$\text{CO}_2^* + \text{H}^* \leftrightarrow \text{COOH}^* + *$	113.1 <sup>[9]</sup>	155.6 <sup>[9]</sup>	77.2 <sup>[10]</sup>	97 <sup>[8]</sup> , 84.9 <sup>[10]</sup>
$\text{CO}_2^* + 2\text{H}^* \leftrightarrow \text{C}(\text{OH})_2^* + 2*$	292.3 <sup>[9]</sup>	217.8 <sup>[9]</sup>		
$\text{CO}_2^* + * \leftrightarrow \text{CO}^* + \text{O}^*$	93.7 <sup>[9]</sup>	169.3 <sup>[9]</sup>	56 <sup>[10]</sup>	149 <sup>[8]</sup> , 147.6 <sup>[10]</sup>
$\text{COOH}^* + * \leftrightarrow \text{CO}^* + \text{OH}^*$	306.8 <sup>[9]</sup>	308.7 <sup>[9]</sup>	48.2 <sup>[10]</sup>	111 <sup>[8]</sup> , 117.7 <sup>[10]</sup>
$\text{C}(\text{OH})_2^* + \text{H}^* \leftrightarrow \text{CH}_2\text{O}^* + \text{OH}^*$	98.7 <sup>[9]</sup>	125.7 <sup>[9]</sup>		
$\text{CH}_2\text{O}^* + \text{H}^* \leftrightarrow \text{CH}_2^* + \text{OH}^*$	163.7 <sup>[9]</sup>	154.1 <sup>[9]</sup>		
$\text{CO}^* + * \leftrightarrow \text{C}^* + \text{O}^*$	237.4 <sup>[9]</sup>	111.8 <sup>[9]</sup>	290.4 <sup>[10]</sup> , 286.6 <sup>[13]</sup>	206 <sup>[8]</sup> , 153.4 <sup>[10]</sup>
$\text{CO}^* + 2\text{H}^* \leftrightarrow \text{CH}^* + \text{OH}^*$	221.4 <sup>[9]</sup>	146.1 <sup>[9]</sup>		
$2\text{CO}^* \leftrightarrow \text{CO}_2^* + \text{C}^*$	339.6 <sup>[10]</sup>	109 <sup>[10]</sup>	326 <sup>[8]</sup> , 186.2 <sup>[13]</sup>	
$\text{C}^* + \text{H}^* \leftrightarrow \text{CH}^* + *$	69.2 <sup>[9]</sup>	154.1 <sup>[9]</sup>	87.8 <sup>[10]</sup> , 69.5 <sup>[13]</sup>	135 <sup>[8]</sup> , 127.4 <sup>[10]</sup>
$\text{CH}^* + \text{H}^* \leftrightarrow \text{CH}_2^* + *$	68.2 <sup>[9]</sup>	61.9 <sup>[9]</sup>	50.2 <sup>[13]</sup>	26 <sup>[8]</sup>
$\text{CH}_2^* + \text{H}^* \leftrightarrow \text{CH}_3^* + *$	71.4 <sup>[9]</sup>	105.6 <sup>[9]</sup>	48.2 <sup>[13]</sup>	66 <sup>[8]</sup>
$\text{O}^* + \text{H}^* \leftrightarrow \text{OH}^* + *$	137.9 <sup>[9]</sup>	116 <sup>[9]</sup>		82 <sup>[8]</sup> , 97.5 <sup>[10]</sup>
$\text{OH}^* + \text{H}^* \leftrightarrow \text{H}_2\text{O}^* + *$	124.6 <sup>[9]</sup>	99.9 <sup>[9]</sup>	111 <sup>[10]</sup>	89 <sup>[8]</sup> , 86.8 <sup>[10]</sup>
$\text{CH}_3^* + \text{H}^* \leftrightarrow \text{CH}_4 + 2*$	137.4 <sup>[9]</sup>	178.7 <sup>[9]</sup>		129 <sup>[8]</sup>
$\text{H}^* + * \leftrightarrow * + \text{H}^*$	13 <sup>[8]</sup>	13 <sup>[8]</sup>		
$\text{CO}^* + * \leftrightarrow * + \text{CO}^*$	10 <sup>[8]</sup>	10 <sup>[8]</sup>		
$\text{O}^* + * \leftrightarrow * + \text{O}^*$	48 <sup>[8]</sup>	48 <sup>[8]</sup>		
$\text{OH}^* + * \leftrightarrow * + \text{OH}^*$	21 <sup>[8]</sup>	21 <sup>[8]</sup>		

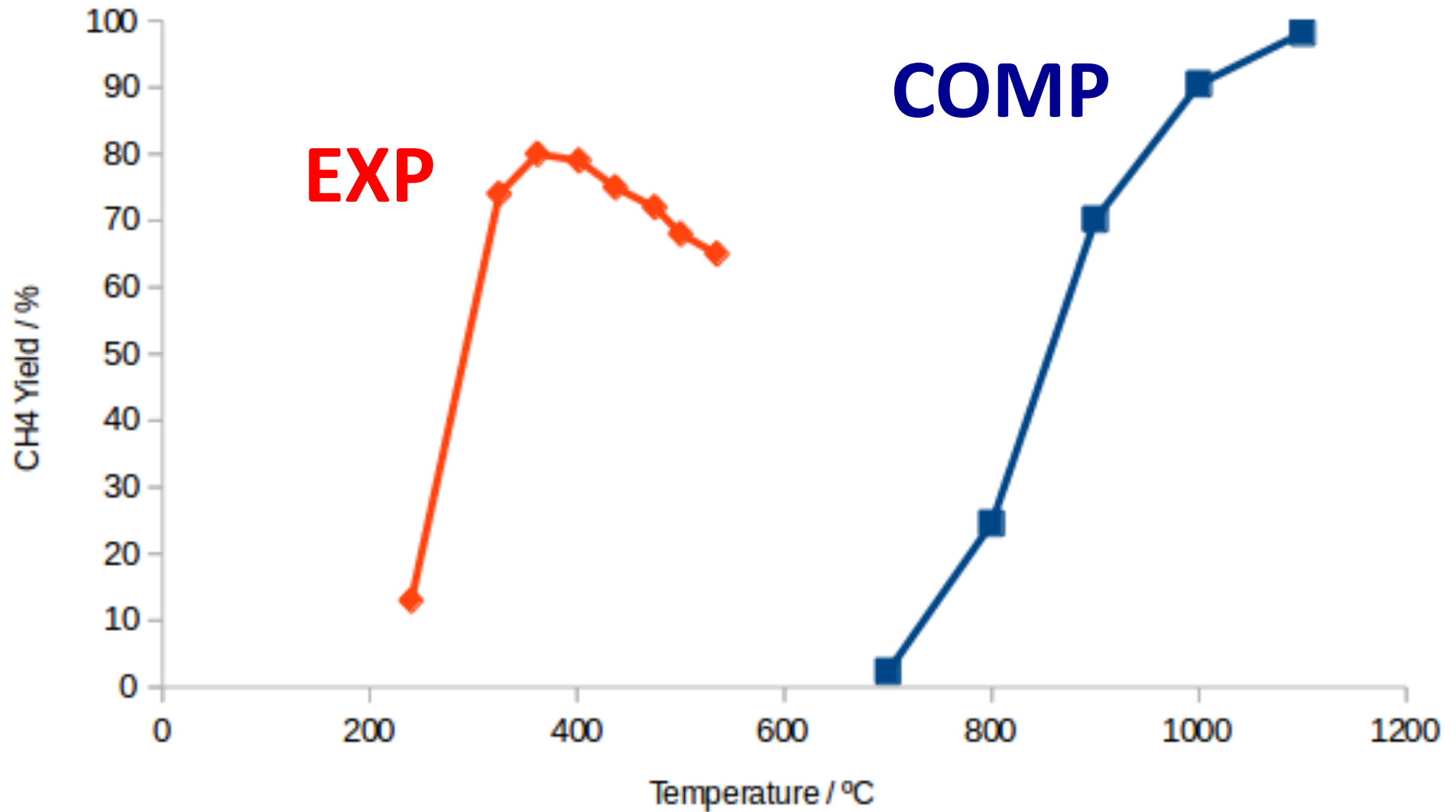
<sup>a</sup>Reverse Energy Barriers were calculated using the equilibrium constant and the forward energy barrier

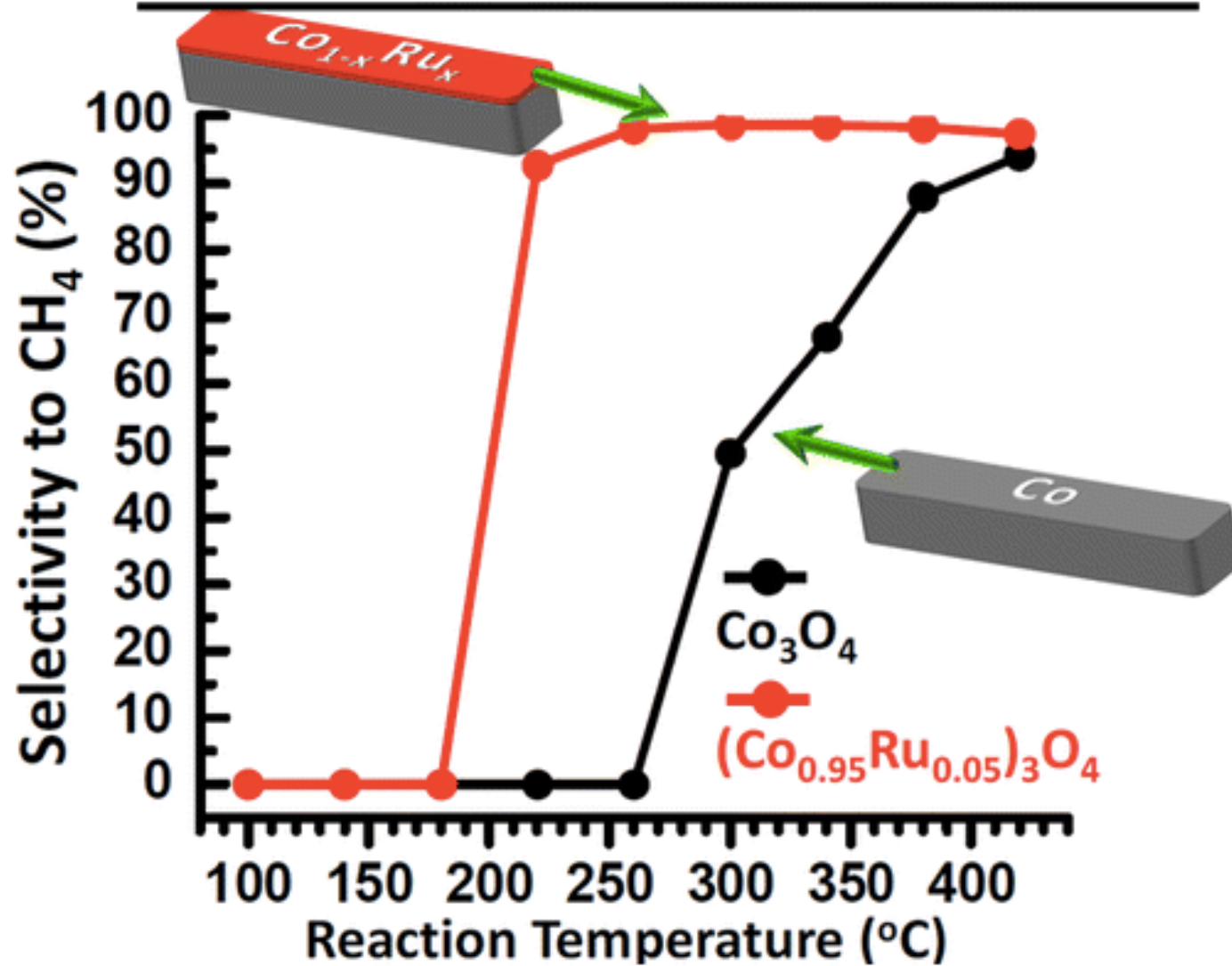
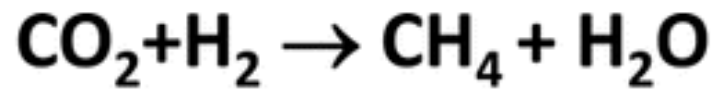
# Results and discussion: % yields



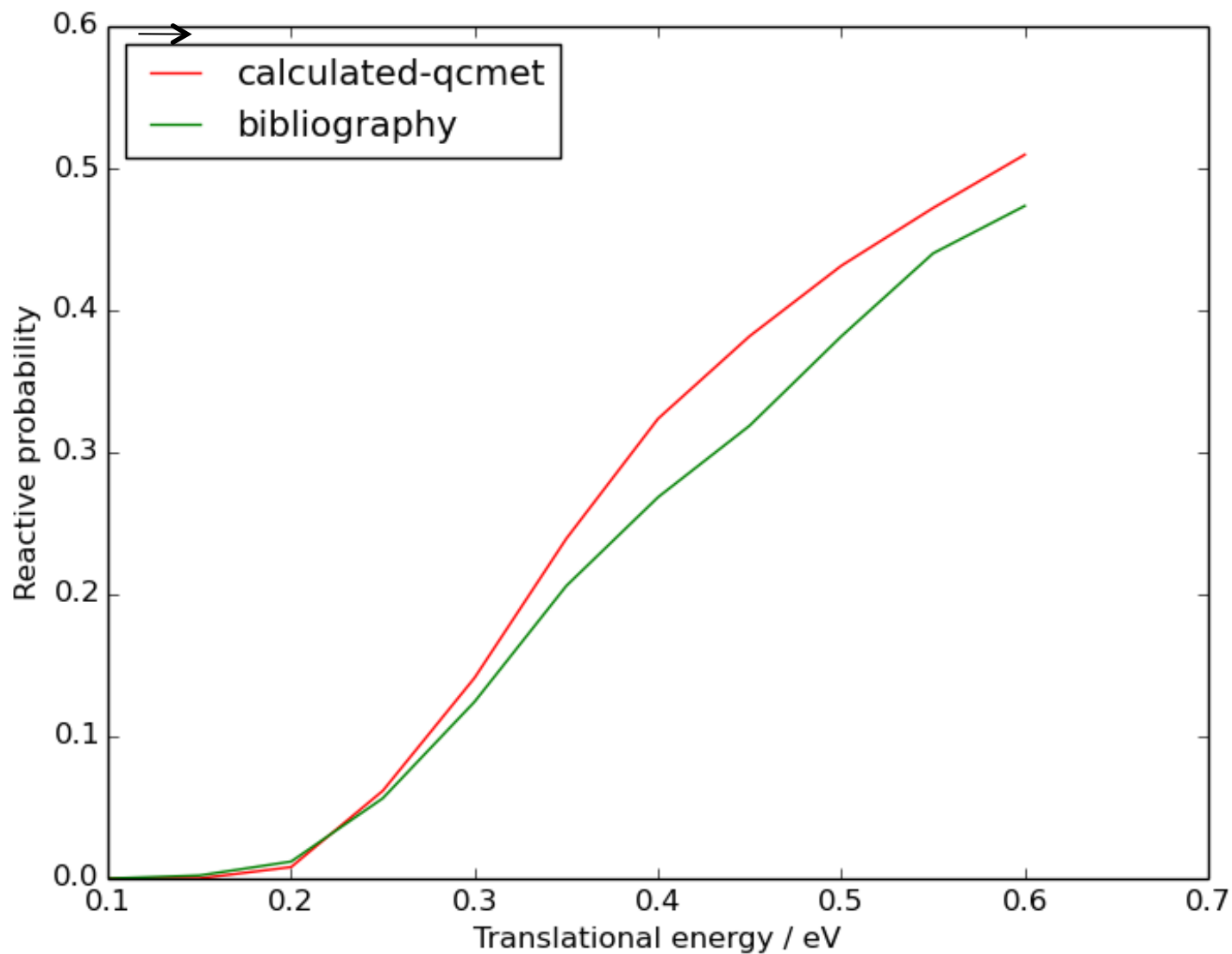


# Results and discussion: CH<sub>4</sub> yield vs T





# Quantum versus Quantum-Classical



# KNOWLEDGE HANDLING: electronic tests

## European Chemistry Test

Core Chemistry Evaluation

The map shows Europe with various countries highlighted in shades of orange and yellow. Labels for different languages are placed over the map, corresponding to the countries where the test is available. The languages listed are: Bulgarsko, Cesky, Dansk, Deutsch, Eësti, Ellinika, English, Español, Français, Italiano, Latviska, Lietuvu, Magyar, Nederlands, Norsk, Polski, Português, Română, Russki, Slovensko, Suomi, and Svenska.

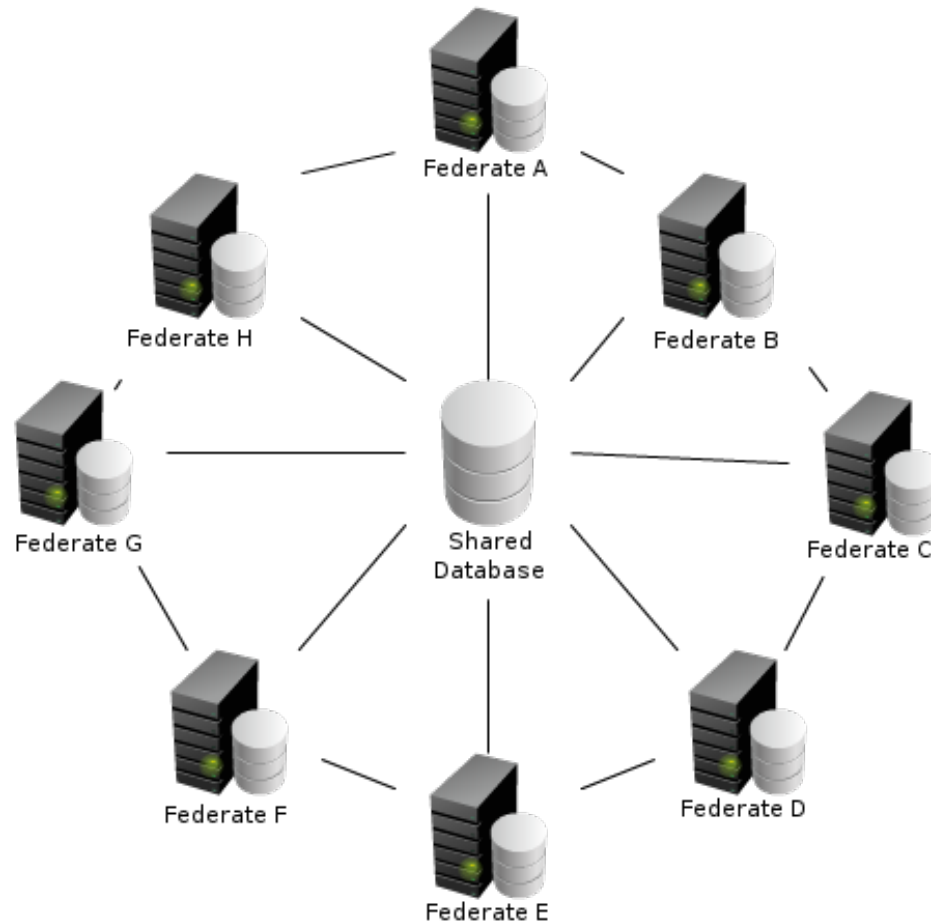
The logo for the European Chemistry Thematic Network (ECTN) is located in the top right corner. It features a blue square with a white border, containing the text "European Chemistry Thematic Network" around the perimeter and "ECTN" in the center, surrounded by yellow stars.

640 x 480  
256 colours

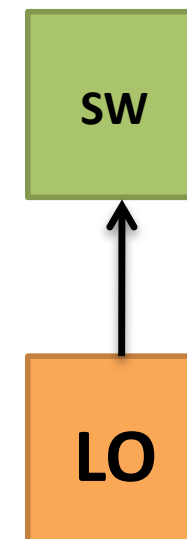
ECTN © 1997-2001

[www.EChemTest.net](http://www.EChemTest.net)

# KNOWLEDGE HANDLING: distributed repository

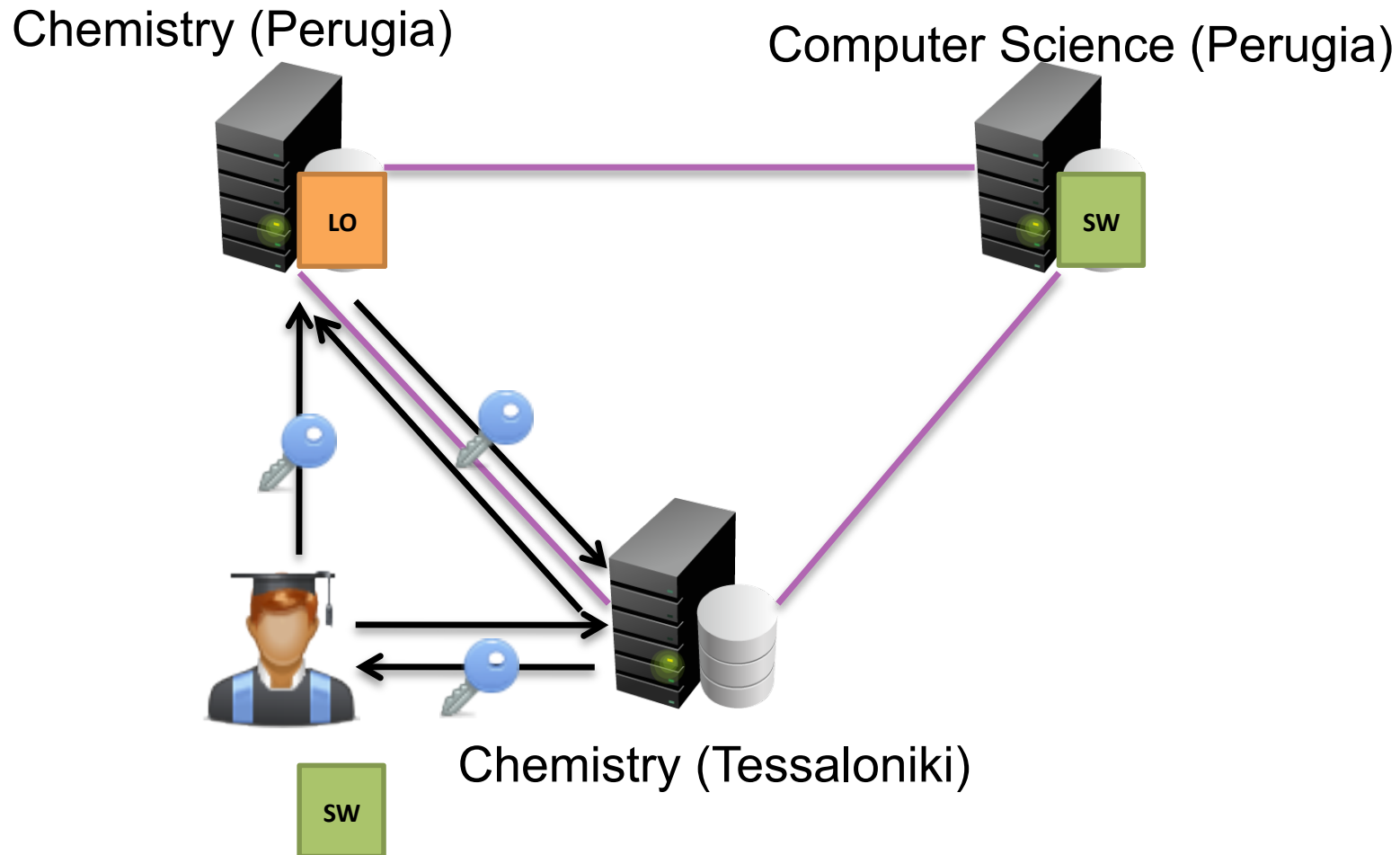


- Federation of autonomous repositories
- Automatic content sharing
- Downloadable content (for registered users)
- Simplified content import from Moodle
- LO Dependency management



# A three site use case

S. Tasso, S. Pallottelli, M. Rui, E. Varella, A. Lagana, *Learning Objects Efficient Handling in a Federation of Science Distributed Repositories*, **Lect. Notes Comp Science, 2013, 2014**



# OTHER COMPETENCE LINES

- engineering technologies of reactors and electrolysers (ENEA, RPC)
- Methane storage as Clathrate hydrates (UNIPG, UB)
- Efficient generation of electricity (ENEA, UNIPG)
- KNOWLEDGE Handling (ENEA, MUP, ECTN, BCO)