The SMARTCATs COST Action

CHEMISTRY OF SMART ENERGY CARRIERS AND TECHNOLOGIES: A EUROPEAN COST NETWORK

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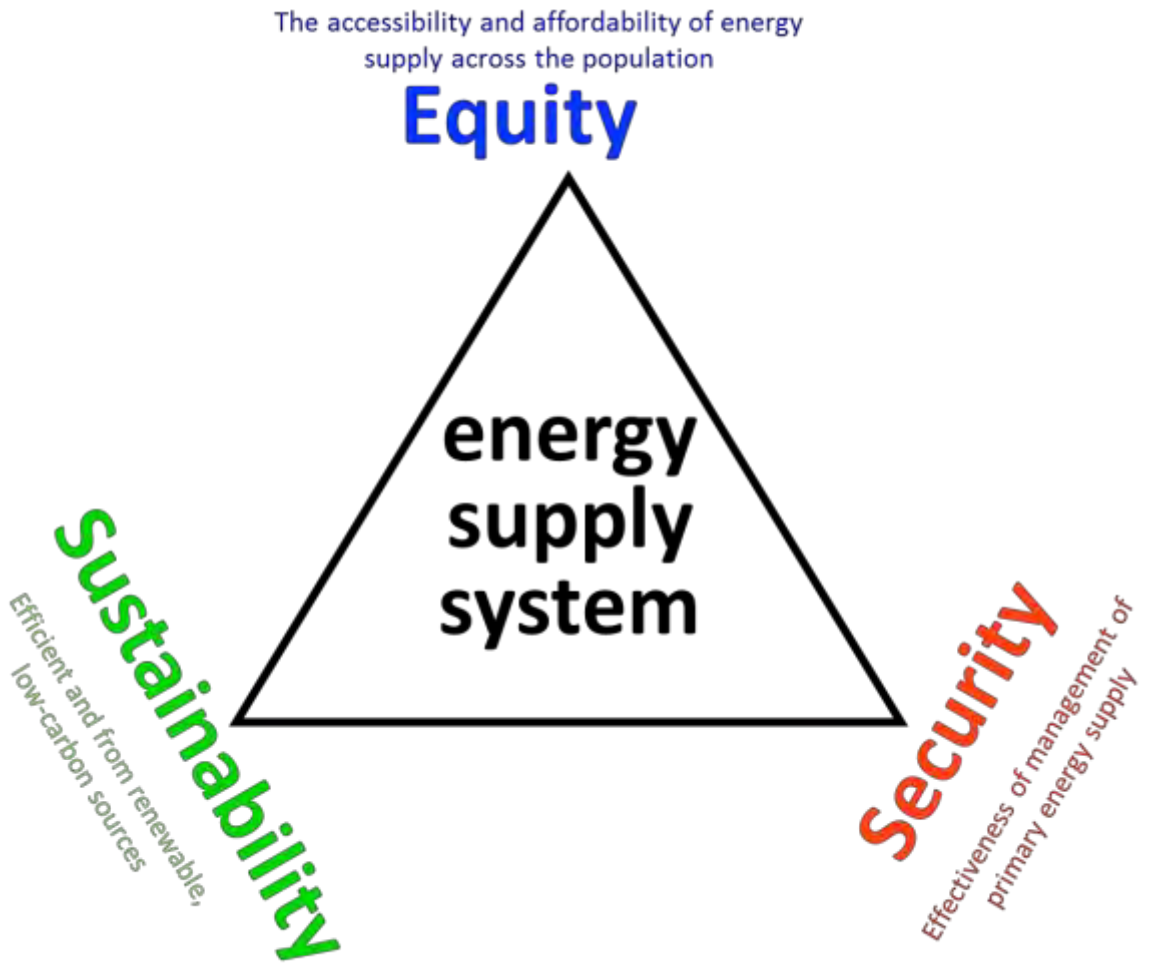
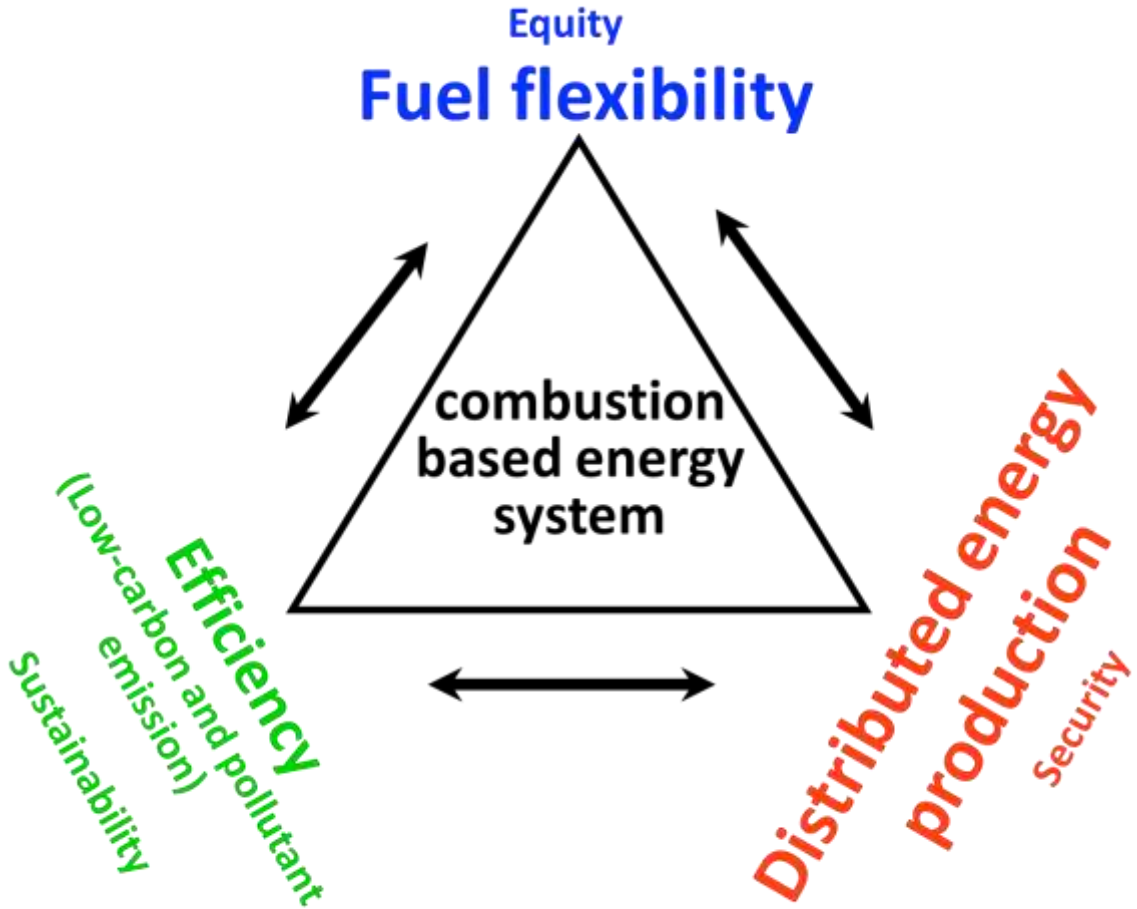
SMARTCATs
2nd General Meeting
&
Workshop on Smart Energy Carriers in Industry

The Energy Trilemma



The Combustion Trilemma



- A new energy production and distribution system based on smart grid concepts and utilizing Smart Energy Carriers (SEC).
- SECs are conventional and novel energetic molecules from conventional or alternative (re)sources selected on the basis of their best-available production and/or utilization technologies.
- SECs are strong candidates as possible solutions for energy storage, transfer and transformation from renewable (local) sources (wind, solar, biomass, waste).

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Smart Energy Carriers (SECs)

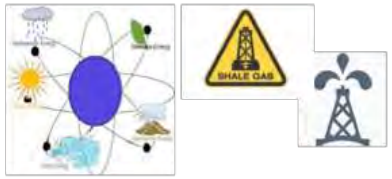
novel AND conventional energetic molecules

and many others ....

increasing in number and typology

deriving from

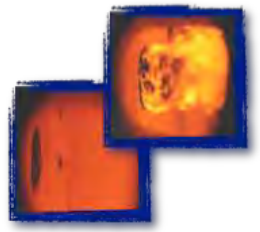
alternative or conventional (re)sources



increasing in number and typology

advanced processes and technologies

H_2 enriched gas turbines



SECs features:
exploiting many and diverse sources
providing the most suitable energy mix for the end-use technology
energetically and CO_2 efficient on the basis of used technologies

The SMARTCATs COST Action aims to set-up a Europe-wide network of leading academic and research institutions and key industries to promote the use of smart energy carriers on a large scale in order to increase fuel flexibility and carbon efficiency of energy production and to support distributed energy generation strategies.

The SMARTCATs COST Action

In line with EU objectives & H2020

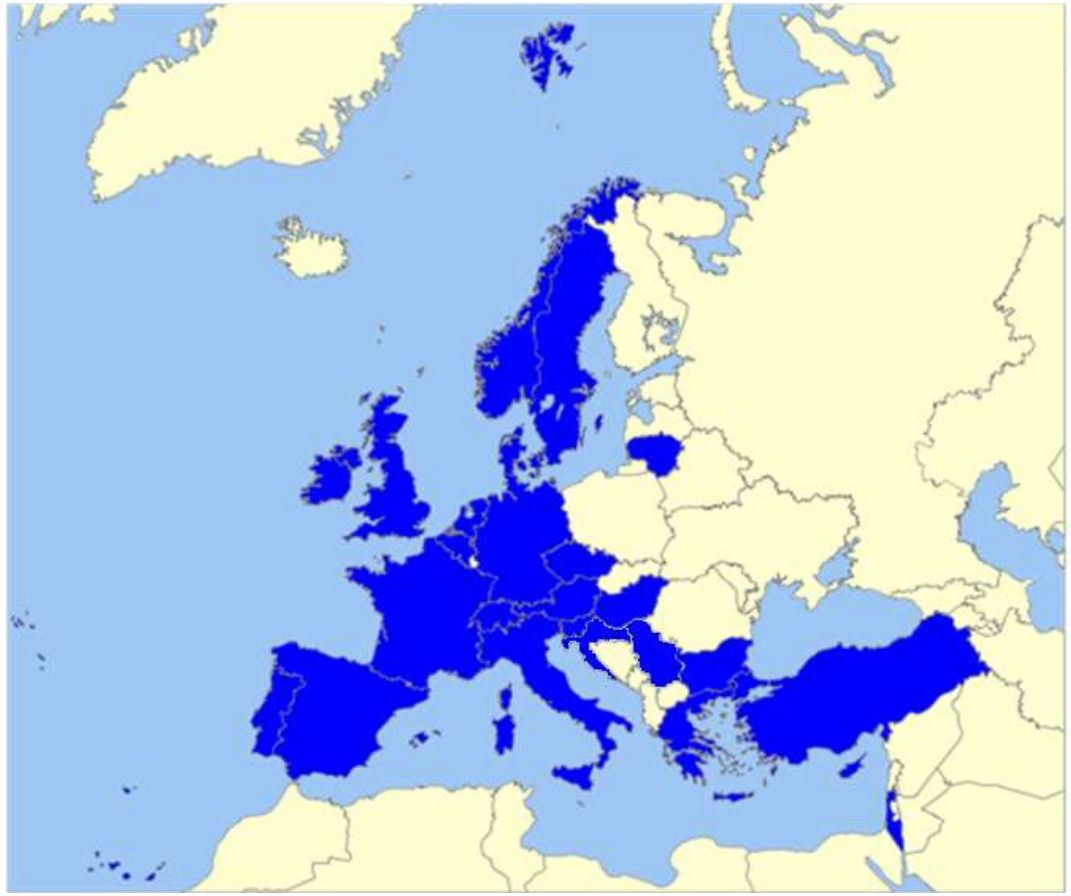
Synergies with Competitive low-carbon energy, Energy efficiency, Mobility for growth

In line with the challenged-based approach of H2020.

Strong and active industrial co-operation will help bridge the research and innovation divide

SMARTCATS STRATEGIC VISION

The SMARTCATs COST Action



A total of 75 organizations from 25 participating countries (EU and Associated States) plus the US, China and Brazil. Strong industrial participation

The SMARTCATs COST Action

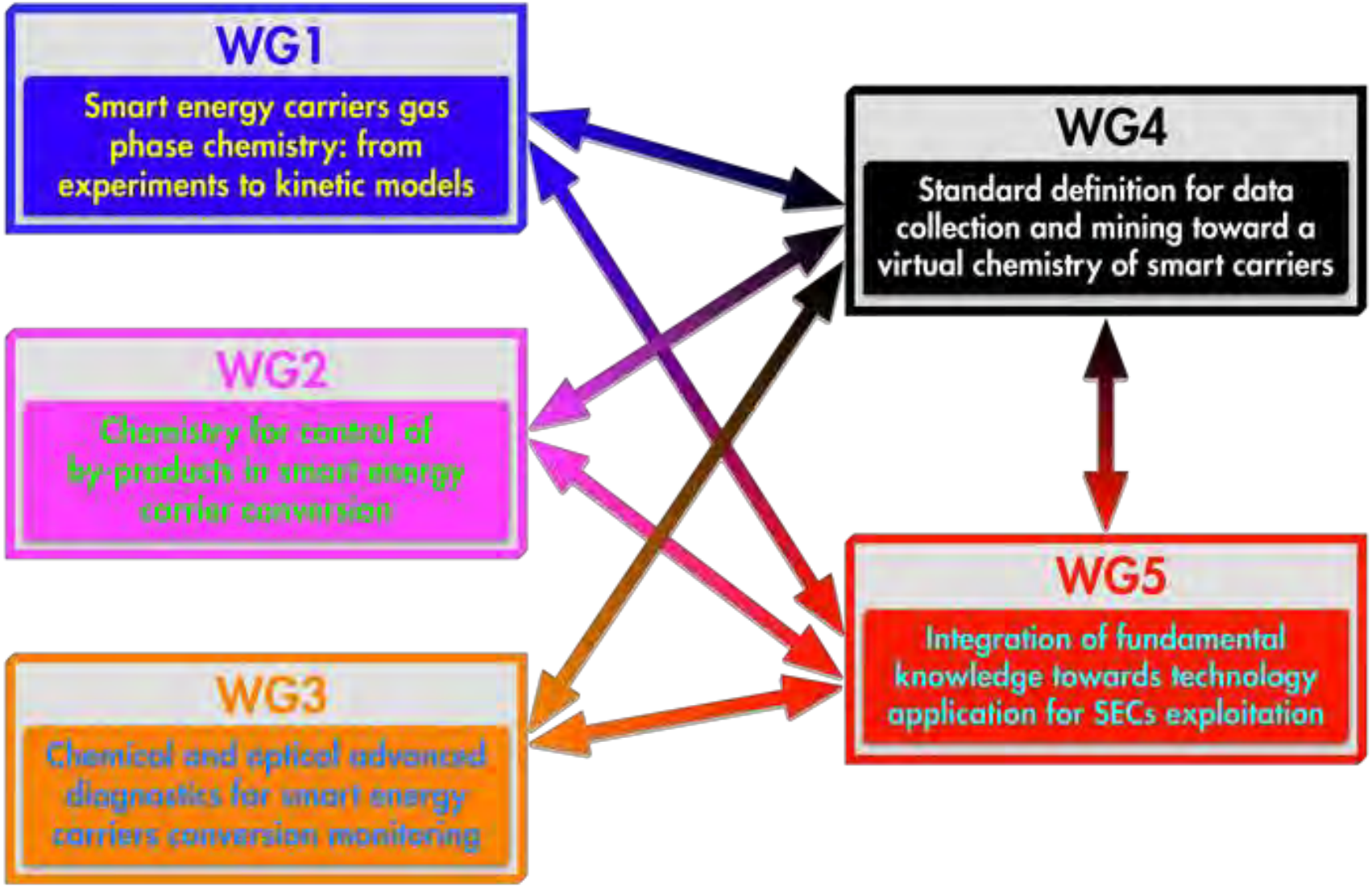
Key dates

Grant Agreement: November 2014

Start of Action: March 2015

End of Action : March 2019

The Working Groups

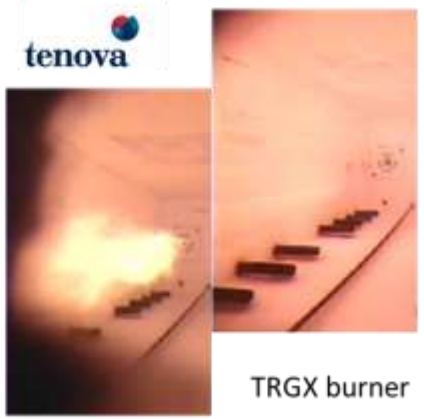


The Working Groups – WG1

AIM: Improve knowledge on detailed chemistry and thermochemistry for pyrolyis, oxidation and combustion of SECs

- New molecules
- Modified interaction
- New working conditions ranges (new technologies - higher pressures (>40-50 bar), low temperatures)

→ *small changes can lead to huge differences* →



TRGX burner

New kinetic models AND improved effectiveness of existing models

Natural gas mixtures (compressed or liquefied natural gas, syngas, bio-natural gas containig also large amout of CO_2 and H_2O)

Simple molecules present in 1st and 2nd generation biofuels (large normal and iso-paraffins, alcohols, esters, saturated and unsaturated cyclic ethers (e.g derivate from furane))

Lignocellulosic biomasses components and molecules derived from their degradation (e.g gamma-valerolactone)

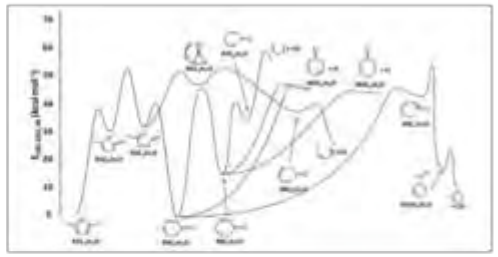
Complex mixtures found in 1st and 2nd generation biofuels (such as Fatty Acid Methyl Esters, Hydrogenated Vegetal Oil or in the proposed surrogates)

The Working Groups – WG1

Modeling

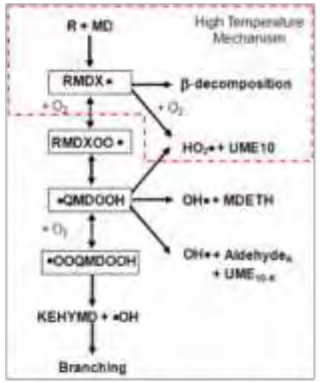
- Automatic generated mechanisms (large molecules)
- Simplification procedures (e.g. lumping)
- Theoretical evaluation of
  - thermodynamic parameters
  - Modern quantum chemical methods (e.g. coupled cluster methods, density functional theory)
  - kinetic parameters
  - Statistical theories (RRKM theory, statistical adiabatic)
- Uncertainty analysis (critical for the use of such models within the engineering design process)

Bielefeld University - CNRS



Dimethyl furan decomposition pathway

Politecnico di Milano



Experiments

Temperature, pressure, composition

CNRS - DCPR

Laminar flat flame burner at low pressure

Karlsruhe Institute of Technology

Shock tube

National University of Ireland

Rapid compression machine

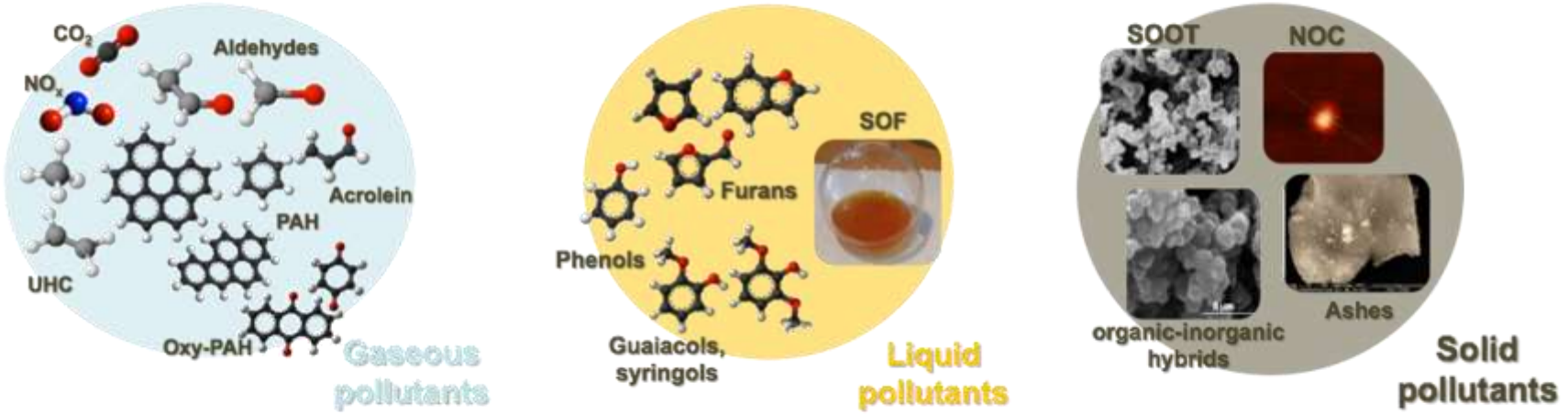
from microscale .... *to macroscale*

The Working Groups – WG2

AIM: increase the knowledge on the formation of organic and inorganic combustion by-products in order to improve the sustainability of SECs.

New "fuels" + New technologies = "New" pollutants (oxygenates, soot, etc)

new operative conditions
new interactions



- Development of more accurate chemical models for pollutants – fundamental experiments
- Development of inventory of noxious emissions from combustion devices (conventional vs alternative fuels)

The Working Groups – WG2

Approachs and tools

- Experiments: gaseous, liquid and solid pollutants

University of Zaragoza

Flow reactor

Istituto Superior Técnico

Drop tube

tenova

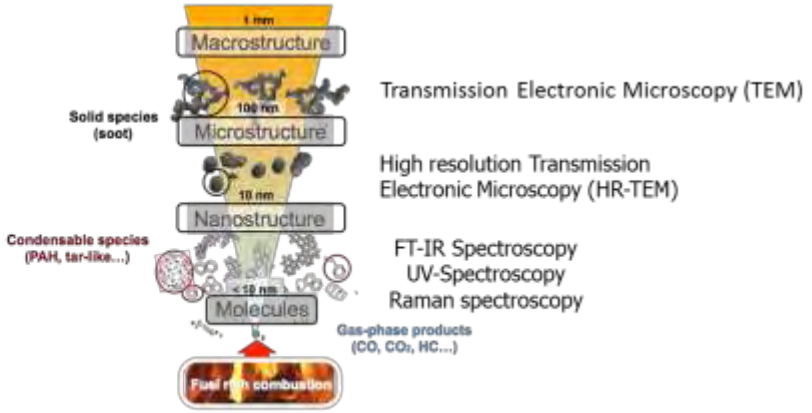
1-Digit Burner Prototype

from microscale → *to macroscale*

- Modeling: gaseous pollutants and particle formation and growth

- Solid characterization

AFM of nanoparticles



The Working Groups – WG3

AIM: provide a forum for the development and evaluation of diagnostic tools and procedures ranging from elementary reaction rate determination to real time measurements in practical devices.

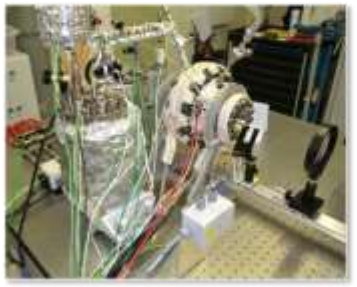
FOCUS

Advanced sampling and chemical analysis coupled with laser-based and mass-spectrometric diagnostics → *Simple combustion devices and chemical kinetics experiments* →

Time and species resolved analysis of combustion processes

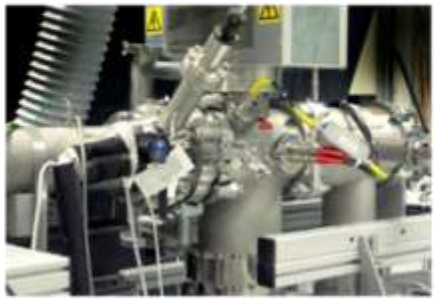
Elementary chemical reactions

Fluid-dynamics/chemical-kinetics interaction



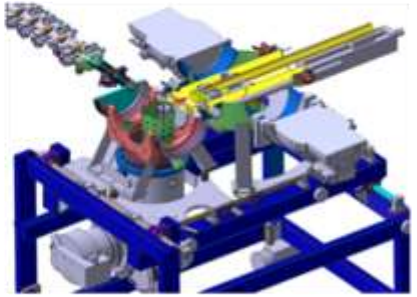
Technische Universität-Freiberg (Germany)

Time Resolved Mass Spectrometry



University Duisburg-Essen (Germany)

Photo-Electron Photo-Ion COincidence spectroscopy



PSI-Villingen (Switzerland)

Laser Induced Fluorescence for radical detection in flame

University of Lille (France)

The Working Groups – WG3

PERSPECTIVE

Identification of suitable markers of combustion progress and efficiency

*Evaluation of diagnostic tools in "**harsh**" conditions*

→

Diagnostic capability transfer from fundamental to complex systems

→

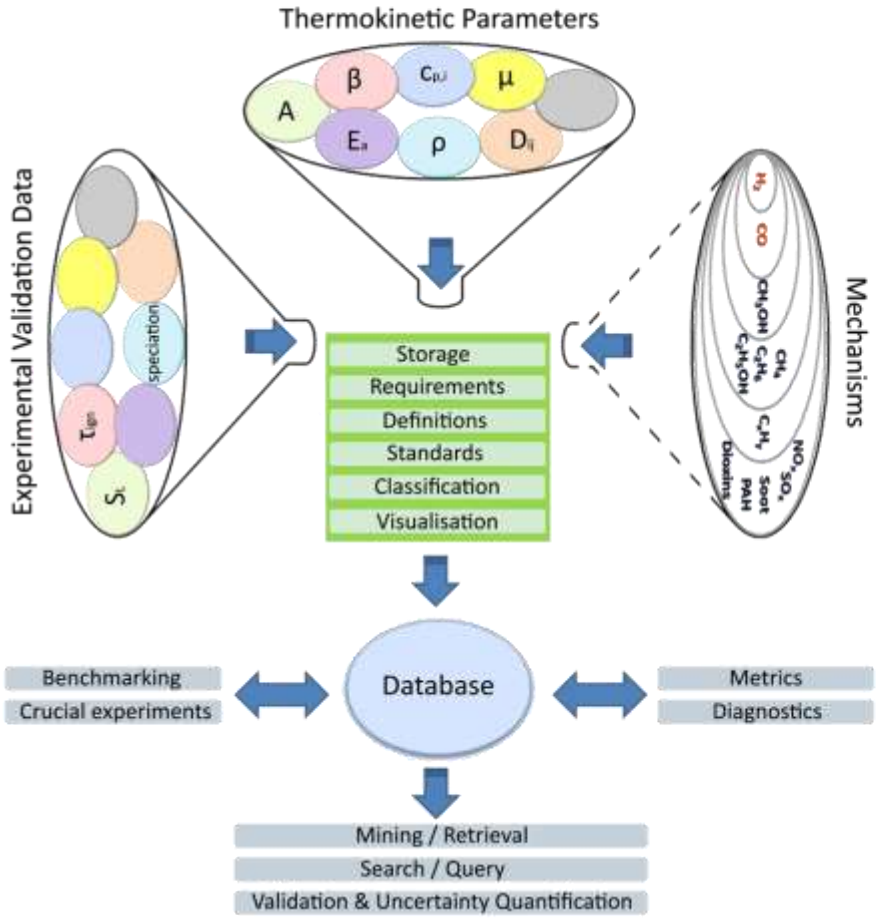
Combustion and emission measurements in complex systems:Engines, Furnaces, Boilers, Household appliances ...

↓

Identification of possible markers and sensors for implementation of ICT monitoring and control systems

The Working Groups – WG4

AIM: identification of the main requirements and tools for the development of databases, software and mathematical tools for data collection and handling as well as chemistry optimization using data mining techniques.



Main Challenge:

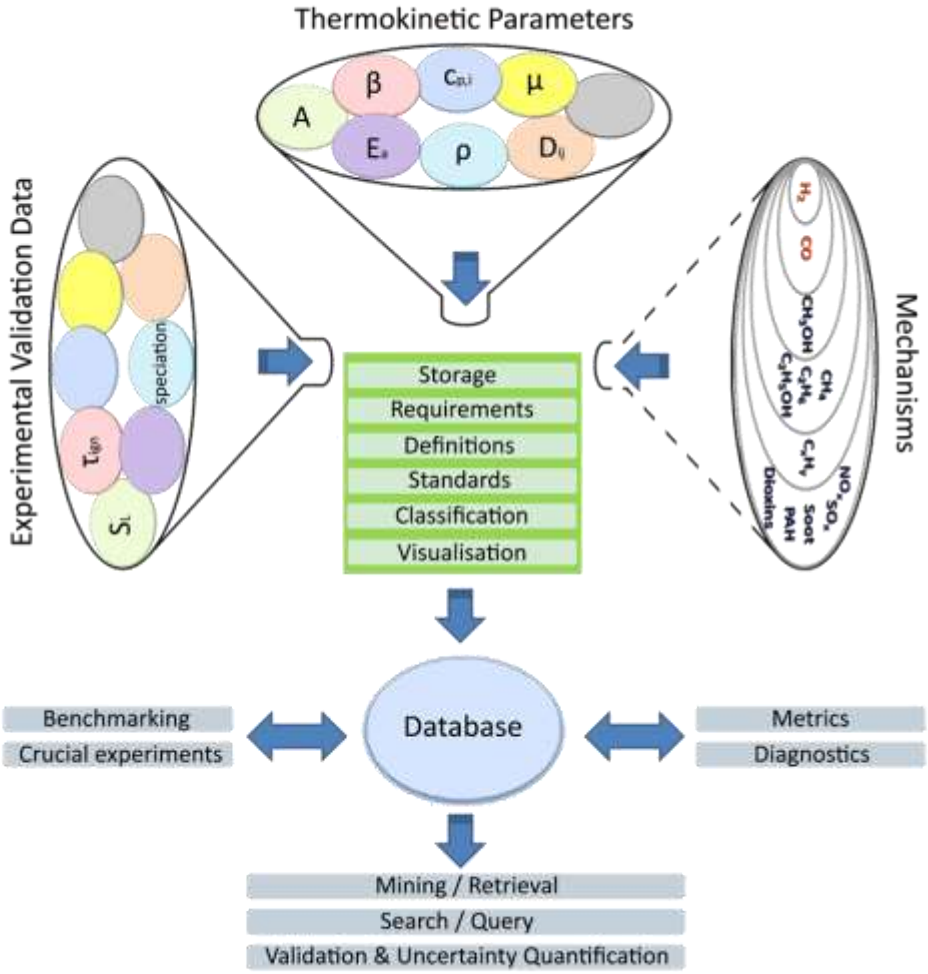
provide a forum for all experts in the combustion community to formulate a common set of requirements for a universal combustion database:

-capable of efficiently store the vast amount of raw data generated by experiments and modeling

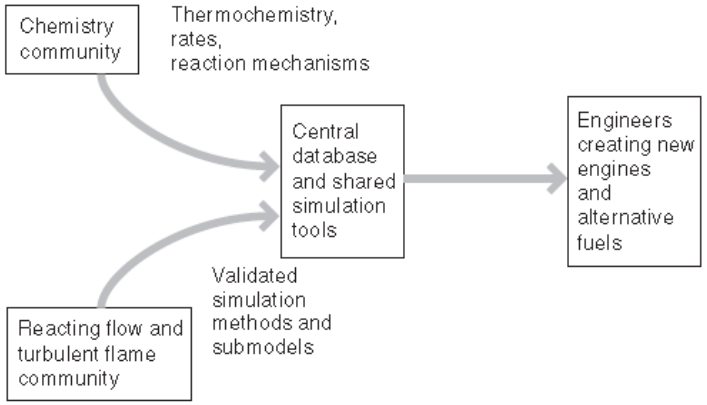
-efficiently accessible for future use and maintenance.

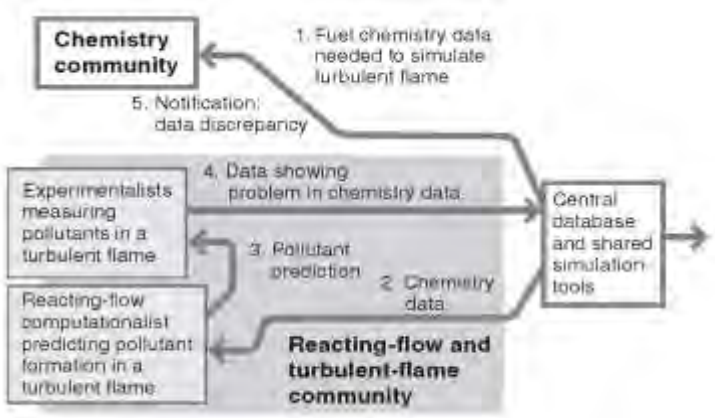
The Working Groups – WG4

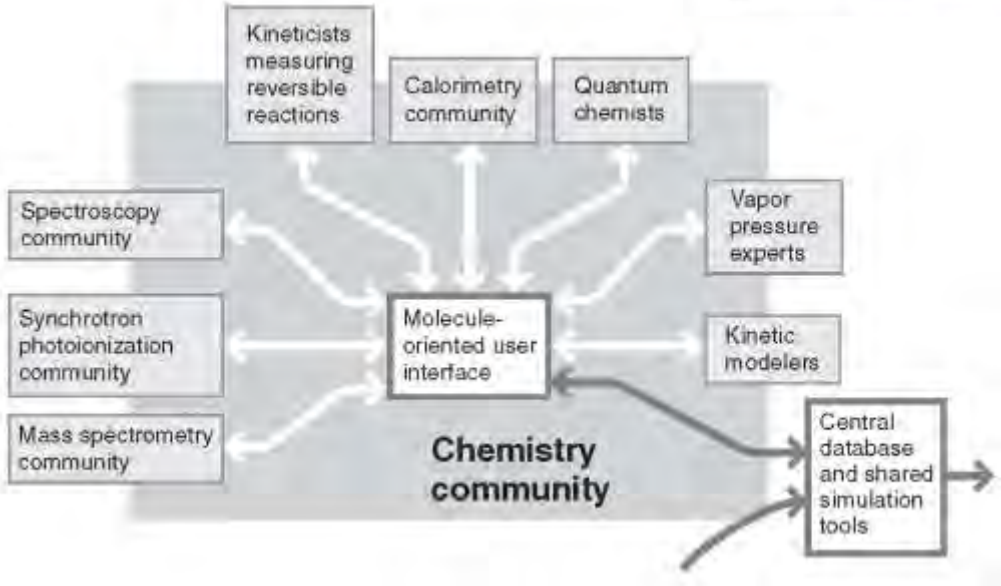
- *Definition of **specific sets of prerequisites** and goals for the establishment of a combustion database that will allow efficient electronic communication of combustion-related data.*
- *Definition of **critical raw, experimental and numerical data** that needs to be made available for the evaluation and possible future re-evaluation of derived parameters and the format required for their efficient communication.*
- *Definition of **crucial experiments** needed to provide a consistent match between experimental evidence and model validation*
- *Active discussion and research involving the sensitivity and establishment of **error bounds both in experimental data and modeling results**.*
- *Development of **methods**, such as those from data mining, to analyze the vast quantities of already existing data in order to provide new insight into the combustion process.*



The Working Groups – WG4







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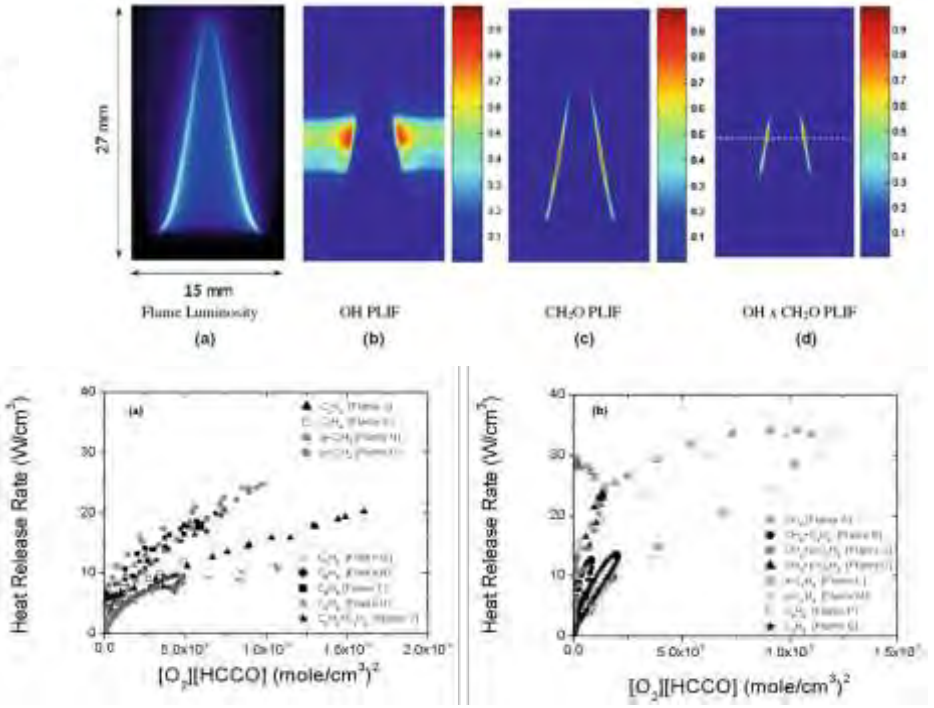
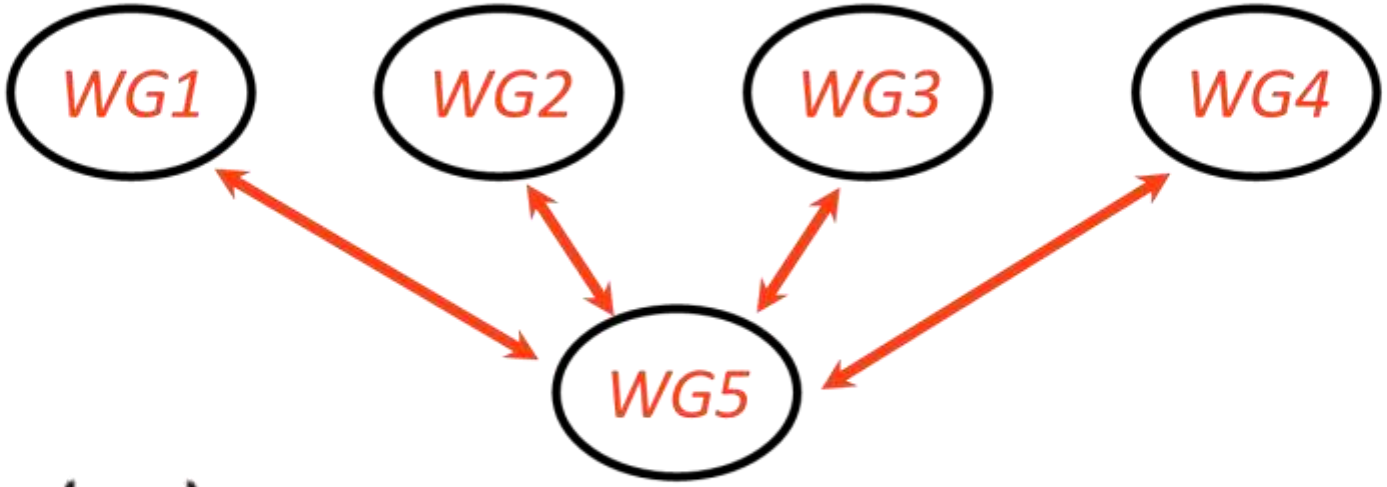
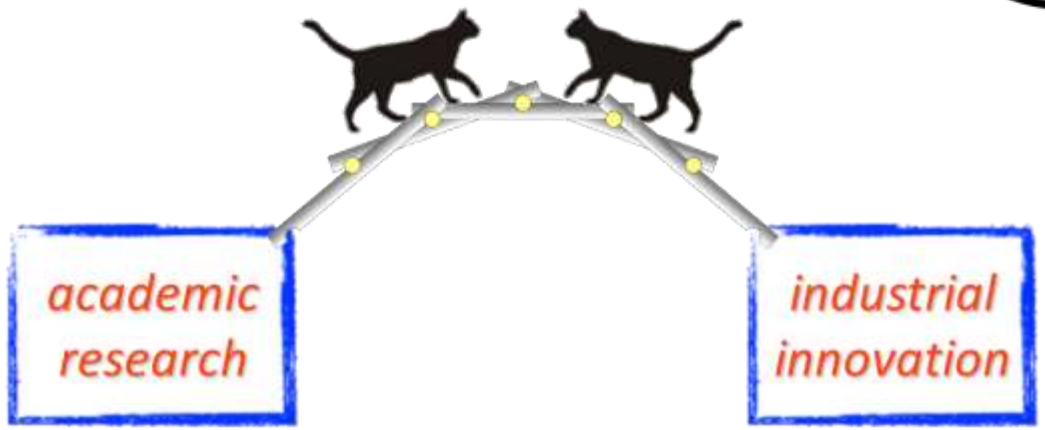


Heat release markers for the combustion of alternative aviation fuels in gas turbines (Skevis et al., 2nd ECATS Conference)

The Working Groups – WG5

AIM: provide optimized ready to use tools and techniques for an effective use of SECs on large scale.



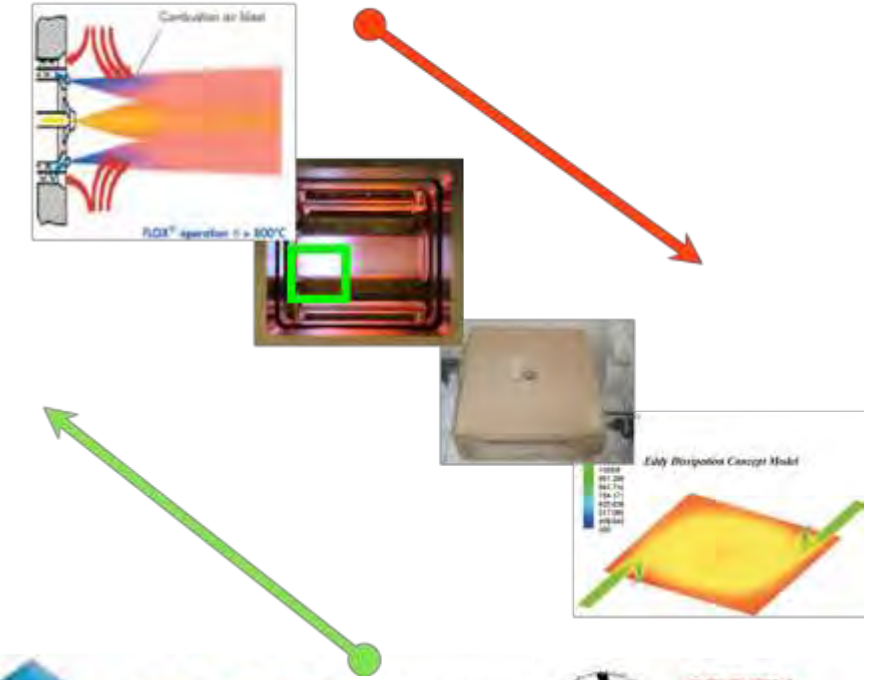


bridge the research-innovation gap

The Working Groups – WG5

- Integration of detailed kinetic mechanisms in large scale numerical simulations
- Development/optimization of reliable, widely applicable and affordable turbulence/chemistry interaction models
- Assessment of the uncertainty related to numerical predictions for their use in new design and regulation

→ taking into account the typology of combustion regime and the features of target technology



The SMARTCATs COST Action

NETWORKING TOOLS

- **Workshops, meetings, conferences**

  Meetings are organised in any COST country participating in the network. They can be of different types, such as Management Committee meetings, Working Group Meetings, Workshops and Conferences. They are open to the whole scientific community and provide visibility opportunities for the COST Action. COST contributes to the travel and subsistence costs of participating scientists, and to the organisation costs of the meeting (**1st SMARTCATs General Meeting, Thessaloniki, Greece, 8/2015, Workshop on Smart Energy Carriers for Power, Industry and Engines, Thessaloniki, Greece, 8/2015, 2nd General Meeting, Lisbon Portugal, 11/2016, Workshop on Smart Energy Carriers in SMEs, 11/2016**)

- **Training schools**

  Training Schools provide intensive training in emerging research topics within the laboratories and organisations involved in the COST Action. Participants are mainly, but not exclusively, young researchers involved in COST Actions. (**Workshop on Data Collection and Mining toward Virtual Chemistry of Smart Energy Carriers, Napoli, Italy, 4/2016**, **Training school on uncertainty analysis of SECs kinetic mechanisms, Budapest, Hungary, 6/2015**).

- **Short Terms Scientific Missions**

  Short-term scientific missions (STSM) are exchange visits between researchers involved in a COST Action, allowing scientists to visit an institution or laboratory in another COST country. They are aimed at fostering collaboration, sharing new techniques and infrastructure that may not be available in other participants' institutions or laboratories. STSM are intended especially for young researchers.

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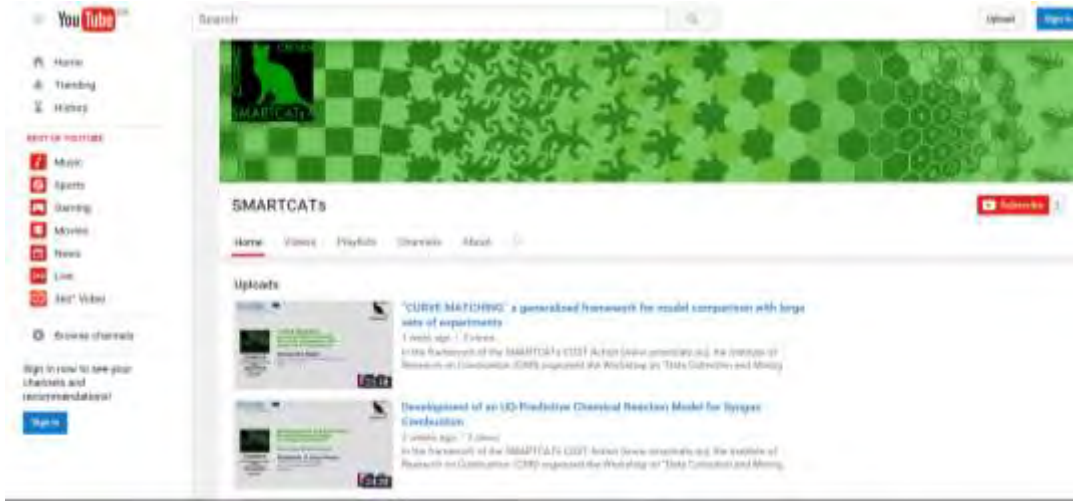

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