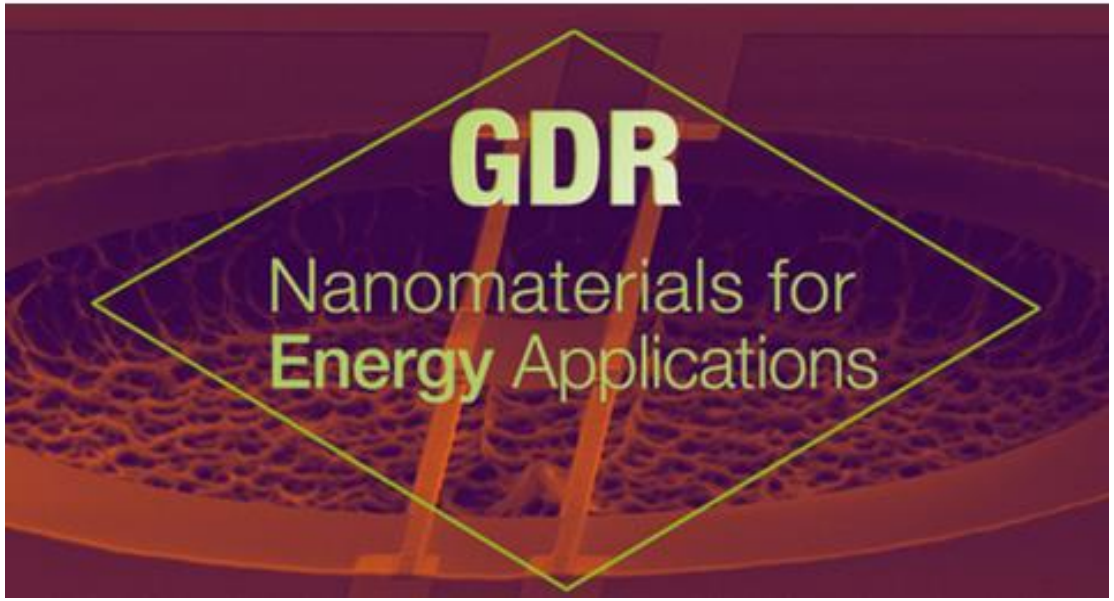
NAME

GDR Nanomaterials for Energy Applications



Working group 1: Nanomaterials-Nanostructuration

Animators: Séverine Gomès, Fabien Grasset, Samy Merabia, François Piquemal

CETHIL UMR 5008 | Institut des Sciences Chimiques de Rennes UMR CNRS 6226 | iLM Institut Lumière Matière | Laboratoire National de Métrologie et d'Essais LNE

GDR2086

cnrs

Plenaries 4-6 October 2021

Overview

- **« Nanomaterials for energy application »**
  definition for the GDR

- **The four essential elementary scientific and technological bricks** to produce nanomaterials for Energy applications

- **Brief reminder of results from workshops**

- **Main conclusions and perspectives**

- **Current projects and calls about Nanomaterials for energy**

Round table

/ François Piquemal

Nanomaterial Definition

In ISO/TS 80004, nanomaterial is defined as the "*material with any external dimension in the nanoscale or having internal structure or surface structure in the nanoscale*", with nanoscale defined as the "*length range approximately from 1 nm to 100 nm*". This includes both nano-objects and nanostructured materials, which have internal or surface structure on the nanoscale.

Nano-objects

nanoparticle

nanofiber

nanoplate

nanorods

nanotubes

nanoribbon

One-dimensional nanostructures

2D materials

nanocristaux

Nanostructured materials

nanocomposite

nanofoam

nanoporous material

nanocrystalline material

3D nanomaterials

...

PROPOSITION: 100 nm → sub-micronic

Do you agree with this proposition?

Energy application

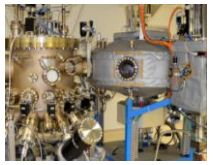
WG3: Energy Conversion

WG4: Thermal Management

WG5: Energy Storage Microdevices

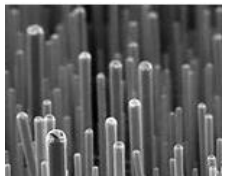
WG6: Micro-Nano-Devices

Four scientific topics



a. Elaboration-Synthesis

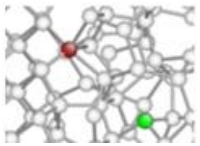
- Real nanomaterials and synthesis processes



b. Measurements techniques for microstructural definition

- Characterized nanomaterials and processes

Nanomaterials for Energy applications

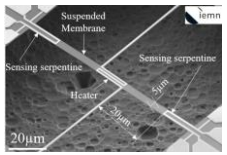


- Design laws at the nanoscales

c. Simulations of energy transport at interfaces and across nanomaterials

- Based on modeling tools and theories available

- Physical property understanding and prediction



d. Measurements techniques of energy transport and conversion properties

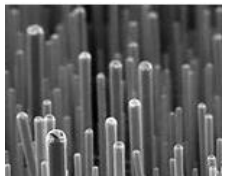
- Physical property understanding and measurement

Comparison validation

Four scientific topics

a. Elaboration-Synthesis

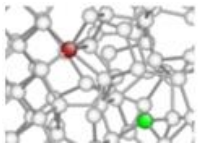
- Real nanomaterials and synthesis processes



b. Measurements techniques for microstructural definition

- Characterized nanomaterials and processes

Nanomaterials for Energy applications

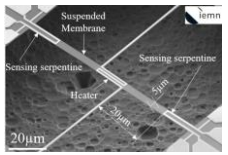


- Design laws at the nanoscales

c. Simulations of energy transport at interfaces and across nanomaterials

- Physical property understanding and prediction

Comparison validation



d. Measurements techniques of energy transport and conversion properties

- Physical property understanding and measurement

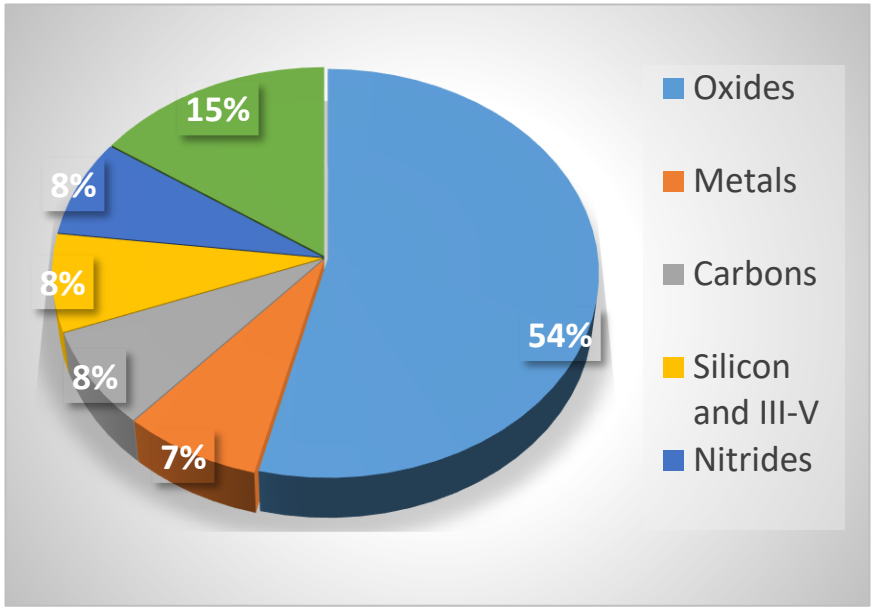
a. Elaboration-Synthesis

From the first workshops

→ **a very broad variety of compounds and nanomaterials seems to be available in the GDR Name.**

"Elaboration-synthesis" processes two main parts:

- **Vacuum (or low partial pressure control) processes**
- **non-vacuum processes.**



Nanoparticles, Nanorods, 2D, Nanocomposites, Thin films …

Piezoelectrics, Pyroelectrics, Thermolectrics, Electrochromism, Catalysis…

Necessity to be in relation and connected with all others workshops !

a. Elaboration-Synthesis

White paper

Contributions : 50%

1.2 Elaboration-Synthesis

1.2.1. Introduction – Definition

1.2.2 Vacuum (or low partial pressure control) processes

- Oxides
- III.V

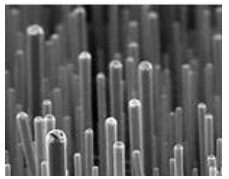
1.2.3 Non-vacuum processes

- Oxides
- Metals
- Carbon and graphene
- Chalcogenides, Nitrides

Four scientific topics

a. Elaboration-Synthesis

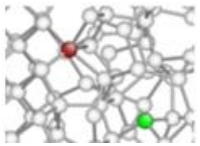
- Real nanomaterials and synthesis processes



b. Measurements techniques for microstructural definition

- Characterized nanomaterials and processes

Nanomaterials for Energy applications

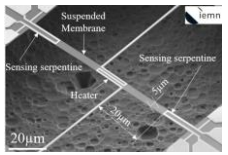


- Design laws at the nanoscales

c. Simulations of energy transport at interfaces and across nanomaterials

- Physical property understanding and prediction

Comparison validation



d. Measurements techniques of energy transport and conversion properties

- Physical property understanding and measurement

b. Measurement techniques for microstructural definition

Starting an Overview on characterization techniques of structural and chemical properties

- ✓ X-ray analysis (GIXRF, SIMS etc)
- ✓ Zeta potential measurements
- ✓ Dimensional nanometrology (AFM, SEM …)

⇨ *thickness, roughness, composition, density, depth profile,*

adsorption / desorption, surface fouling, material ageing…

→ Overview to be pursued and completed by most recent techniques or involving hybrid techniques

Need of other contributions!

b. Measurement techniques for microstructural definition

White paper

Contributions : 2/3

1.3 Measurements techniques for microstructural definition

1.3.1 Introduction – Definition

1.3.2 **Advanced methods**

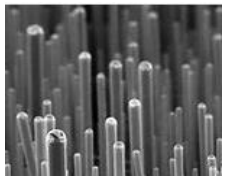
- Combined XRR-GIXRF
- Techniques de Zetamétrie
- Hybrid techniques (exple SEM + AFM, etc)

...

Four scientific topics

a. Elaboration-Synthesis

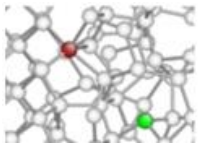
- Real nanomaterials and synthesis processes



b. Measurements techniques for microstructural definition

- Characterized nanomaterials and processes

Nanomaterials for Energy applications

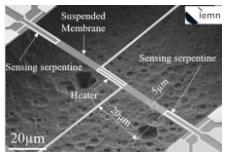


- Design laws at the nanoscales

c. Simulations of energy transport at interfaces and across nanomaterials

- Physical property understanding and prediction

Comparison validation



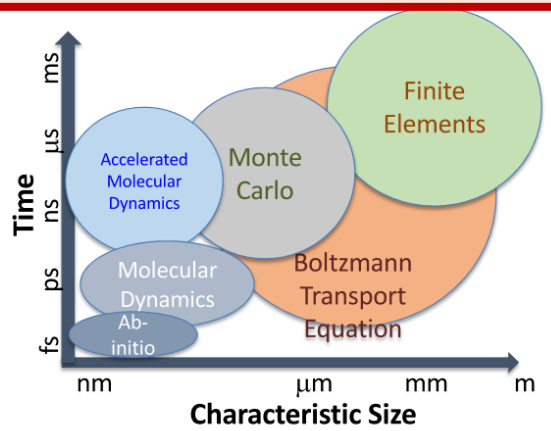
d. Measurements techniques of energy transport and conversion properties

- Physical property understanding and measurement

c. Simulations of energy transport at interfaces and across nanomaterials

Starting an Overview on different simulations techniques

- ✓ Molecular dynamics
- ✓ Ab-initio NEGF calculations
- ✓ Anharmonic Lattice dynamics

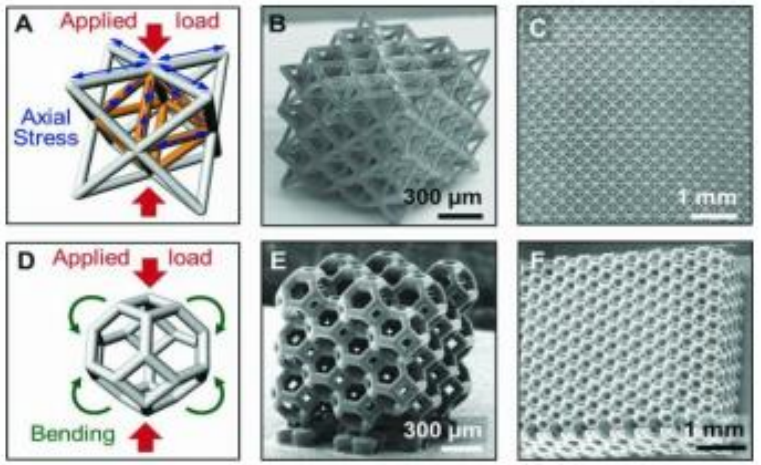


Modeling nanostructured materials: some recent trends

- ✓ Metamaterials
- ✓ Nanostructured interfaces (superlattices, atomic scale films, nanocomposites)
- ✓ Nanowires

Properties

- ✓ Thermal conductivity
- ✓ Nanoscale friction



c. Simulations of energy transport at interfaces and across nanomaterials

Elementary processes at interfaces and across nanomaterials

- Interfacial thermal resistance and phonon transmission
- Electron and electron-phonon processes
- Effect of the interface roughness and defects

Simulation techniques (to compute the behavior of carriers at interfaces)

- Non Equilibrium Green's function (NEGF)
- Non Equilibrium Molecular dynamics (NEMD)
- Approach to Equilibrium (AEMD)
- Wave packet simulations
- Monte-Carlo/ BoltzmannTransport Equation (MC-BTE)

Applications

Thin films, Superlattices, Nanocomposites, Phononic crystals, Nanoporous materials…

White paper

Contributions : 1/5

Which properties?

c. Simulations of energy transport at interfaces and across nanomaterials

Perspectives

- nanofluidic systems
- electron-phonon coupling in nanostructures
- phonon-photon coupling

Subfields not represented

- Behaviour of energy carriers at interfaces: electrons, phonons, photons
- Electronic transport in nanostructures,
- Polymers, SAMs, molecular junctions

Interactions/synergy with other workshops

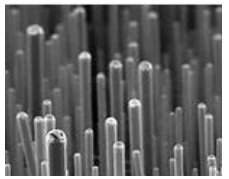
- Atelier 2: de la description des processus fondamentaux aux systèmes nanostructures :

How to play with nanostructuration to modulate the behaviour of energy carriers d'énergie: filtering, cooling, couplings

Four scientific topics

a. Elaboration-Synthesis

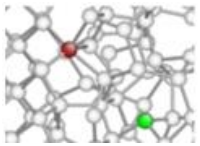
- Real nanomaterials and synthesis processes



b. Measurements techniques for microstructural definition

- Characterized nanomaterials and processes

Nanomaterials for Energy applications

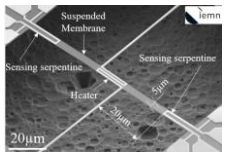


- Design laws at the nanoscales

c. Simulations of energy transport at interfaces and across nanomaterials

- Based on modeling tools and theories available
- Physical property understanding and simulation

Comparison validation



d. Measurements techniques of energy transport and conversion properties

- Physical property understanding and measurement

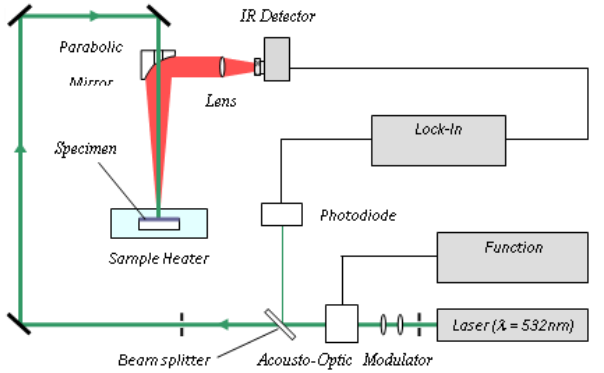
d. Measurements techniques of energy transport and conversion properties

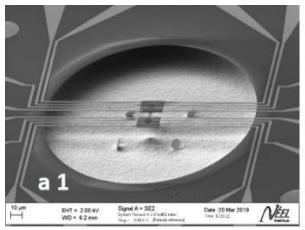
Starting an overview on different measurement techniques

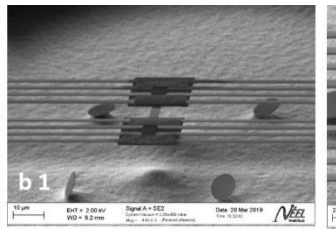
✓ **Thermal methods**

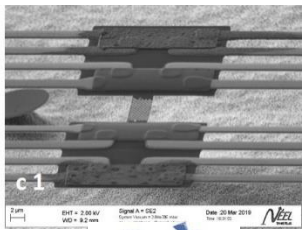
- Photothermal methods *(Frequency domain photothermal radiometry (PTR))*
- Electrothermal methods
- Scanning thermal microscopy

Thermal conductivity, diffusivity, effusivity, barrier resistance, surface phonon-polaritons heat transfer, heat flux, specific heat









✓ **Electrical methods**

- Atomic force microscopy-based techniques

Electric current, voltage, surface potentiel, Work function, barrier height , electrical resistance, capacitance and conductance, Dopant concentration

✓ **Measured nanomaterials**

- 3D thin films and bulk substrates
- 2D membranes and thin films
- 1D nanowires

Need of other contributions!

d. Measurements techniques of energy transport and conversion properties

1.5.1 Thermal properties and parameters

- Photothermal methods
- Electrothermal methods
- Atomic Force Microscopy based thermal methods
- Near-field optical Microscopy based thermal methods
- Electron microscopy based thermal methods

1.5.2 Electrical properties and parameters

- SPM based techniques

...

1.5.2 Thermoelectric properties and parameters

1.5.3 Optical properties and parameters ?

1.5.5 Mechanical properties and parameters ?

1.5.4 Chemical properties and parameters ?

White paper

Contributions : 2/5

Which properties?

Main conclusions

- A very broad variety of compounds and nanomaterials available
- Requirements in terms of thermal characterization

- Overviews started on:
  - synthesis methods
  - recent techniques or hybrid techniques for microstructural and chemical characterization
  - simulations techniques
  - measurement techniques

Need of other contributions!

- Which physical properties and parameters ?

- Necessity to be in relation and connected with others workshops.

Call for contributions

a. Elaboration-Synthesis

- Amorphous compounds (glasses…)
- Polymers

b. Measurements techniques for microstructural definition

- Advanced methods

c. Simulations of energy transport at interfaces and across nanomaterials

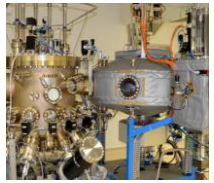
- Behaviour of energy carriers at interfaces
- Electron transport in nanostructures,
- Amorphous materials,
- Polymers

Which properties and parameters ?

d. Measurements techniques of Energy transport and conversion properties

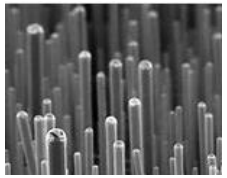
- Thermoelectric properties and parameters
- Optical properties and parameters ?
- Mechanical properties and parameters ?
- Chemical properties and parameters ?

Which properties and parameters ?



a. Elaboration-Synthesis

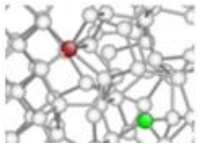
- Real nanomaterials and synthesis processes



b. Measurements techniques for microstructural definition

- Characterized nanomaterials and processes

Nanomaterials for Energy applications

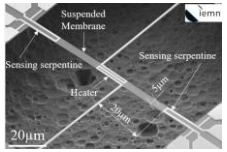


- Design laws at the nanoscales

c. Simulations of energy transport at interfaces and across nanomaterials

- Based on modeling tools and theories available

- Physical property understanding and prediction



d. Measurements techniques of Energy transport and conversion properties

- Physical property understanding and measurement

Comparison validation

Expected input from Axis 2 due to modelling and theory limitations from other Axes regarding nanomaterial property specification

Expected input from other axes regarding nanomaterial property specification

WG1: Nanomaterials and nanostructuration

WG2: Transport Properties at the Nanoscale

How to play on nanosctructuration to tune the behavior of energy carriers: filtering, cooling, couplings?

Which properties to be simulated and measured at the level of the nanomaterial?

WG3: Energy Conversion

WG5: Energy Storage Microdevices

WG4: Thermal Management

WG6: Micro-Nano-Devices

Which properties to be simulated and measured ?
at the level of the nanomaterial? or at the level of the devices?
What are the expectations and the needs?

From WG3, analyzed energy conversion

- **Conversion « Thermal ⇔ Electrical »**
- **Conversion « Optical ⇔ Electrical »**
- **Conversion « Mechanical ⇔ Electrical »**
- **Conversion « Chemical ⇔ Electrical »**
- **Hybrids / Cogeneration …**

Properties and parameters to be considered?

- **Thermal** conductivity, diffusivity, flux, resistance, heat capacity , temperature,…
- **Electrical** electrical resistivity, I V curve, permittivity …
- **Thermoelectric** Seebeck effect, electrical resistivity, thermal conductivity, Peltier coefficient
- **Optical** emissivity, reflectivity, properties of absorption and fluorescence
- **Mechanical** displacement, deformation, flexibility, stiffness, friction…
- **Chemical** electrochemical properties, ionic retention, catalyze kinetic
- **…**

Perspectives

- **Continuing the overviews on:**
  - **synthesis methods**
  - **recent techniques or hybrid techniques for microstructural and chemical characterization**
  - **simulations techniques**
  - **measurement techniques**

➡ White paper

- **Second meeting on nanoscale thermal metrology** in collaboration with the club nanometrology by the end of the year

Traçability, interlaboratory comparison …

Club nanoMétrologie

*__Initiated action__: for **nanoscale electrical metrology by SPM techniques**

Proposal of action:

Based on the specification requirements for Energy applications,
→ to identify “Model” nanomaterials (composition, size, shaping…) to propose new compounds or devices.

For example, an idea could be to launch calls to prepare a given compound by different techniques and compare the impact of the synthesis method on the properties.

Current projects and calls about Nanomaterials for Energy

The list is non exhaustive !

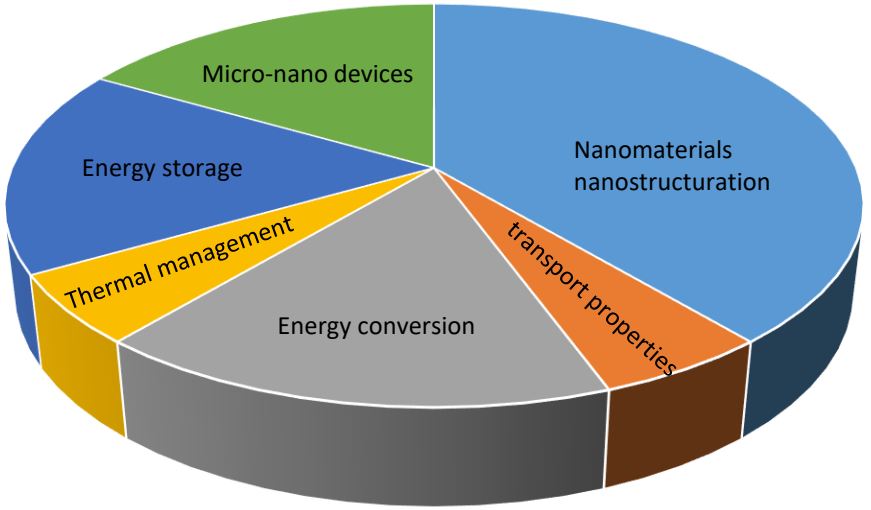
With the help of Nolwenn Fleurence and Khaled Kaja !

H2020

14 on-going projects

EMPIR (European Metrology Program for Innovation and Research)

6 on-going projects



Current projects and calls about Nanomaterials for Energy

The list is non exhaustive !

H2020

NanoBat GHz nanoscale electrical and dielectric measurements of the solid-electrolyte interface and applications in the battery manufacturing line

PeSD-NeSL Photo-excited State Dynamics and Non-equilibrium States under Laser in Van der Waals Stacked Two-dimensional Materials

LEE-BED Innovation test bed for development and production of nanomaterials for lightweight embedded electronics

SAbyNA Simple, robust and cost-effective approaches to guide industry in the development of safer nanomaterials and nano-enabled products

ELECNANO Electrically Tunable Functional Lanthanide Nanoarchitectures on Surfaces

NaMeS "Interdisciplinary NAnoscience School: from phenoMEnology to applicationS"

NANOthermMA Advanced Simulation Design of Nanostructured Thermoelectric Materials with Enhanced Power Factors

Current projects and calls about Nanomaterials for Energy

The list is non exhaustive !

H2020

ASTERIQS Advancing Science and TEchnology thRough dIamond Quantum Sensing

FLATLIGHT Functional 2D metamaterials at visible wavelengths

ESTEEM3 Enabling Science and Technology through European Electron Microscopy

HybridSolarFuels Efficient Photoelectrochemical Transformation of CO2 to Useful Fuels on Nanostructured Hybrid Electrodes

MEMS 4.0 Additive Micro-Manufacturing for Plastic Micro-flectro-Mechanical-Systems

HARVESTORE Energy HarveStorers for Powering the Internet of Things

REACTION first and euRopEAn siC eigTh Inches pilOt liNe

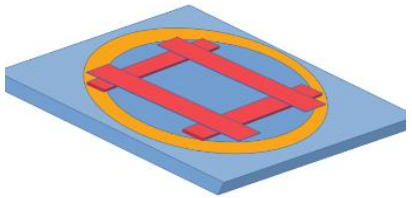
Current projects and calls about Nanomaterials for Energy

2019 Call EMPIR:

19ENG05 nanoWires: High throughput metrology for nanowire energy harvesting devices
https://www.ptb.de/empir2020/nanowires/home/

***Aim**: To map the performance and conversion efficiency of NW energy harvesting devices and to link their overall properties with those of individual nanowires (NWs).*

19ENG06 HEFMAG: Metrology of magnetic losses in electrical steel sheets for high-efficiency energy conversion
https://hefmag.inrim.it/



One of the objectives is to study and model power losses in thin sheets within a DC-MHz frequency regime, with the help of fluxmetric, magneto-optical characterisation techniques as well as scanning probe techniques for the sub-µm regime.

19NRM04 ISO-G-SCoPe: Standardisation of structural and chemical properties of graphene

The overall aim of this project is to validate and standardise measurement and characterisation methods for the chemical and structural properties of graphene in powders and liquid dispersions for industrial applications.

→ energy sector, photovoltaics, lithium ion batteries

Current projects and calls about Nanomaterials for Energy

2020 Call EMPIR:

20IND04 ATMOC Traceable metrology of soft X-ray to IR optical constants and nanofilms for advanced manufacturing

The overall objective of the project is to develop traceable measurement techniques for optical constants of thin-film systems and nanostructures and to use these techniques to support the introduction of an improved optical properties database for industrial users.

20IND08 MetExSPM: Traceability of localised functional properties of nanostructures with high speed scanning probe microscopy

The overall objective of this project is to design and develop technologies for transforming HS-SPM (~10 mm/s) metrology instruments for use in industrial high-speed quantitative multi-sensing metrology with a target traceable position measurement uncertainty of 1 nm.

20IND12 Elena: Electrical nanoscale metrology in industry

http://projects.lne.eu/jrp-elena/

The overall objective of the project is to establish a European metrological infrastructure and cost-effective technologies for C AFM and SMM to allow industry to conduct traceable measurements of electrical properties on materials and devices at the nanoscale.

Network

European Metrology Network 19NET01 AdvManuNet:
Support for a European Metrology Network on advanced manufacturing

This project aims to strengthen the European position in advanced manufacturing by accelerating the development and uptake of innovative metrology, by focusing on the needs of advanced manufacturing and optimising stakeholder interaction with the metrology community.

Among the defined Key industry sectors of this network:

- ✓ Energy generation, transmission and storage
- ✓ Advanced materials (incl nano-enhanced materials) and processing
- ✓ Nano- and microtechnology (nanowires …)
- ✓ Optics and photonics (nanoLED …)

Solar panel manufacturing

https://www.euramet.org/research-innovation/search-research-projects/details/project/support-for-a-european-metrology-network-on-advanced-manufacturing/?tx_eurametctcp_project%5Baction%5D=show&tx_eurametctcp_project%5Bcontroller%5D=Project&cHash=901958111e7a8f77ea640901483f349e

Future calls

European Partnership on Metrology (EPM)

2021 Green Deal
2022 Health, Integrated European Metrology
2023 Fundamental, Industry
2024 Green Deal
2025 Health, Integrated European Metrology
2026 Fundamental, Industry
2027 Green Deal

- Normative and some form of Research Potential in each year

Budget ambition: 700 M€
210 M€ of EU money for internal funded partners
140 M€ of EU money for external funded partners
National cofunding of 350 M€

JRP ≈ 2 – 3 M€
Ext funded ≈ 40 %

Current projects and calls about Nanomaterials for Energy

Future calls

Horizon Europe (HE)

https://ec.europa.eu/info/funding-tenders/opportunities/docs/2021-2027/horizon/wp-call/2021-2022/wp-8-climate-energy-and-mobility_horizon-2021-2022_en.pdf

Workprogramme **2021-2022**
*8. Climate, **Energy** and Mobility*

Batteries and nanoparticles

HORIZON-CL5-2021-D2-01-02: Advanced high-performance Generation 3b (high capacity / high voltage) Li-ion batteries supporting electro mobility and other applications (Batteries Partnership)
HORIZON-CL5-2022-D2-01-02: Interface and electron monitoring for the engineering of new and emerging battery technologies (Batteries Partnership)
HORIZON-CL5-2021-D2-01-04: Environmentally sustainable processing techniques applied to large scale electrode and cell component manufacturing for Li ion batteries (Batteries Partnership)
HORIZON-CL5-2021-D5-01-15: Development and demonstration of cost affordable and adaptable retrofit solutions for tailpipe and brake polluting emissions
HORIZON-CL5-2021-D5-01-16: Assessment of noise and particle emissions of L category vehicles from real driving conditions
HORIZON-CL5-2022-D5-01-07: Prevent smog episodes in Europe: Air quality impact of engine-emitted volatile, semi volatile and secondary particles

https://innovation.engie.com/en/calls-for-projects

Current projects and calls about Nanomaterials for Energy

1) Your experience in European projects ?

Which area? Nanomaterials/nanostructuration, energy conversion, energy storage, thermal management, micro/nano devices

2a) For the submitted projects not funded: What are the main complaints ?

2b) For the funded projects: - What are the main highlights ?
- What are the key impacts ?
- Follow-up ? Conclusion and perspective

3) In the frame of GDR NAME: How can we organise ourselves to propose projects in an efficient way ?