MOLÉCULES ET MATÉRIAUX POUR L'ÉNERGIE DE DEMAIN
MOlecules and Materials for the ENergy of TOMorrow (MOMENTOM)
(Coordinator: Dr. Hynd REMITA)

1. Context, positioning and objectives of the detailed proposal

1.1. Context, social and economic issues

Our societies face the challenge to provide enough global energy while mitigating the climatic constraints. During the recent COP21 many nations have signed the Intended Nationally Determined Contributions (INDCs) to decrease the greenhouse gas emissions and to take actions. It is urgent to put efforts in research and policy to decrease the greenhouse gas emissions and develop renewable energies. Whatever the sustainable energetic mix required for supporting our ever-increasing demands, scientific and technological issues must be cost-effective: scientists must discover materials based on abundant and renewable resources to produce, store and deliver energy. In this quest, advances in material science are enablers for improving energy efficiency in many different areas such as harnessing of solar energy (solar cells), hydrogen technologies, transport (automotive industry and e-mobility), energy efficient buildings, etc.… A recurring problem in energy production and supply is the multi-scale nature of the scientific tasks, from basic research to social and economic aspects of the upcoming technologies. Initiatives (in many countries including USA, Japan, China, Germany, England, Netherland, India, South Africa, Brasil) have launched research programs.
MOMENTOM aims at finding new materials for renewable energies and new strategies to optimise the transition from a carbon-based economy to a sustainable economy. The aspects dealing with the intermittent energy production and grid management are included in the parent IRS project Grid4Earth. Developing new materials and catalysts should be performed along relevant lines for transfer to industrial partners, who will actually implement the change in industrial and domestic energy sources. This is the ultimate goal of MOMENTOM which gathers 26 research laboratories[1] and 10 institutions (CNRS, CEA, Université Paris-Sud, Université Versailles-Saint-Quentin, Université d'Evry, Ecole Polytechnique, ENS Cachan, ENSTA ParisTech, CentraleSupélec, Soleil) within the University Paris-Saclay.[2] Several industrial partners and SMEs have also given a written expression of interest to MOMENTOM (see **annex 2**). This partnership will be of special importance during the project and will open new possibilities for joint research projects or direct support of industrial partners to projects associating MOMENTOM teams. This strategy might therefore ensure a long-term viability to the research impetus provided by MOMENTOM.

1.2. Positioning of the project

MOMENTOM will contribute to the National Strategic Area "Energie propre, sûre et efficace" and the European Energy Challenge (Secure, Clean and Efficient Energy) in H2020. MOMENTOM is located at the heart of the strategy of the University Paris-Saclay (Chemistry department: "The chemistry of the future must be sustainable", in the axis 3 of the Human and Social Sciences Department (SHS)[3] "Land, environment, Energy, food", and transverse actions "Energy" and "Materials"). The project aims at creating the conditions for long-term partnerships between area companies and the Paris-Saclay research teams. It also intends to strengthen the synergies between actors in the field to favour the emergence of international champions.
MOMENTOM stems from discussions among the partners during the last two years which already motivated the organisation of an International Workshop on Materials for Energy (Orsay 18-20th March 2015, 150 participants). MOMENTOM participants belong to the Chemistry Department (67%), the Physics of Wave and Matter Department (PhOM, 22%) the SHS Department (9%), the Life Science Department (SDV) (2%) accounting for 122 researchers. Most of the partners are involved in five LABEX (NanoSaclay, Palm, Charmmmat, LASIPS and MME-DII). MOMENTOM focusses on:
- Development of materials and devices for H_2 production, storage and use,
- Development of a direct conversion of solar energy into chemical energy,
- Development of highly efficient electrical storage materials,
- Economic and social aspects of new energy technologies, such as H_2 or solar energy conversion into fuels.

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[1] LCP, SPMS, ICMMO (ERIEE/LCI), UCP, ILV (EPI/ECHO/SOMO/GEMAC), PPSM, PMC, PICM, IRDEP, LAC, ISMO, LAMBE, SCBM, LPB, LLB, NIMBE, Soleil, LCM, LPS, I2BC, MSSMat, CSNSM, EPEE, CES, CEARC, X (Dept Economy).
[2] The support letters from the heads of the laboratories are in **annex 1**.
[3] The support letter from the Maison des Sciences de l'Homme is in **annex 1**.

The main application field of these technologies concern the transportation and mobile applications, which motivates the support from the MOVEO French Competitivity Center (see letter of support in **annex 2**), MOMENTOM objectives are distinct from those of the above LABEX and local Energy Transition Institutes (ITE). Specifically, MOMENTOM will **NOT** focus on photovoltaic materials per se (because they are at the heart of the ITE IPVF), heat recovery and other industrial processes (targets of the ITE PS2E), neither synthons from CO_2 reduction (topic of LABEX CHARMMMAT).
MOMENTOM is set with a long-term vision to make the University Paris-Saclay a major player in this internationally competitive area. USA has been the precursor in bringing together around 100 world-class scientists and engineers within the Caltech perimeter in the Joint Center for Artificial Photosynthesis in 2010. This Energy Innovation Hub (http://solarfuelshub.org) aims at finding new and effective ways to produce fuels using only sunlight water and carbon dioxide. This initiative gave the impetus for many top American universities [Stanford Global Energy and Climate Project (https://gcep.stanford.edu), MIT Energy Initiative (http://mitei.mit.edu)] to launch their own specific project on energy and climate. MOMENTOM aims at making the University Paris-Saclay a front runner by pursuing the following actions: (i) developing basic and applied research for a faster development of the above technologies, (ii) pursuing technological breakthroughs that would interest industrial partners,[4] (iii) considering economic issues of the energy transition, (iv) settling the conditions for a long-term development of these topics with industrial partners, (v) promoting these new technologies by proposing educational program to both industrial and social partners.

1.3. State-of-the-art and scientific issues

1.3.1. Hydrogen technologies

Hydrogen is considered as a clean energy vector of the future solving the global energy and environmental crises. Development of efficient and cheap materials for green H_2 production is a main challenge towards a sustainable hydrogen economy. However, nowadays hydrogen is produced at 95% from fossil resources, which are limited and CO_2-emitting technologies. The recent growing concerns to the global climate changes due to CO_2 emissions have encouraged the development of new green and renewable technologies to produce hydrogen. In agreement with the "Technology Roadmap: Hydrogen and Fuel Cells"[5], hydrogen is omnipresent in the different energetic and industrial scenarios that are proposed for 2050,[6,7] and mandatory for Europe to respect its commitment to reduce greenhouse gas emissions to 80-95% below 1990 levels by 2050. Hydrogen can be used first to reduce our dependence to fossil resources using wind/solar energy or biomass resources, through electrolysis or biogas reforming, allowing locally producing a CO_2-neutral hydrogen. This hydrogen could then be used in industrial processes or in fuel cells to produce electricity and heat or participate to CO_2-free mobility solutions (70% of the French oil importations). Hydrogen is also an attractive solution to absorb the energy excess produced by renewable resources (30 to 90 TWh at a horizon of 2050, as estimated by the governmental agency ADEME). Therefore, the deployment of hydrogen technologies in synergy with the development of renewable resources is the preferred option at the worldwide level to feed a wide diversity of systems (mobility, heat, industrial processes …). In France, there is a new initiative to promote hydrogen with the big project GRHYD for the city of Dunkerque.
The objective is now to confirm the economic and technical feasibility of the decentralised production and storage of hydrogen from different renewable energy whatever its final use would be. Besides the launching of policies promoting the deployment of the hydrogen-based technologies, research actions are still necessary to give more competitiveness and robustness to the actual devices. This research will concern the whole chain of hydrogen technologies: the H_2 production from renewable sources of electricity or directly from the solar energy, H_2 storage and final use through fuel cells.
Concerning hydrogen production, alkaline electrolysers are currently the most mature technology with investment costs significantly lower than for other electrolyser types. However, Proton Exchange Membranes (PEM) and Solid Oxide (SO) electrolysers have much higher potential for future cost reduction and, in case of SO electrolysers, efficiency improvements. PEM electrolysers show both the highest current density and operational range, prerequisites necessary to reduce investment costs and improve operational flexibility at the same time. **As of today, cell lifetime is a limiting factor for PEM and SO electrolyser**

[4] Letters of support provided in Annex 2, from Big Companies: PSA, Renault, Air Liquide,… ; SMEs : NanoE, NanoMakers, NextMat, TERA environment…
[5] IEA report, « Technology roadmap : hydrogen and fuel cells », 2015
[6] « L'hydrogène dans la transition énergétique », Les avis de l'ADEME, Février 2016
[7] Energy Roadmap 2050, Document N°52011DC0885, European commission, 2011

technologies. Besides, as mentioned in a recent ADEME report on H_2 production, no particular path must be prioritised or excluded. This strategy is also that of the GDR HYSPAC, to which MOMENTOM laboratories will and already participate.
Concerning hydrogen storage, mature options for storage in vessels comprise pressurised and cryogenic tanks, providing hydrogen storage capacities of between 100 kWh (pressurised tanks) and 100 GWh (cryogenic storage). Storing hydrogen in metal hydrides or carbon nanostructures are recognised as promising technology options for achieving high volumetric densities. While metal hydrides are already in the demonstration phase (see McPhyEnergy company), fundamental research is still needed to better understand the potential of carbon nanostructures and will be studied in the MOMENTOM project.
Finally, concerning the fuel cell technology nearest to the end-user, the global market grew by almost 400% between 2008 and 2013, with more than 170 MW of fuel cell capacity added in 2013 alone. Currently, more than 80% of fuel cells are used in stationary applications, such as co-generation, back-up and remote power systems. However, **high investment costs and relatively limited lifetimes remain the greatest barriers to their wider application**.

1.3.2. Direct solar energy conversion into fuels

Beside electrolysis coupled to renewable electricity-sources, MOMENTOM will also explore new routes to hydrogen production based on the direct conversion of solar energy into H_2. In France, there is the new GDR “Solar Fuel” (groupe de recherche supported by the CNRS), which is dedicated to the production of fuels from solar energy. Indeed, solar energy is the most abundant source of clean and renewable energy, but its diluted and intermittent character calls for the development of efficient and economically viable conversion and storage technologies. Depending on applications and targeted power, different solutions can be considered, like the conversion of solar energy into electrical energy by photovoltaic (PV) techniques coupled with storage systems. **An interesting alternative is the transformation of solar energy into chemical energy by photoelectrochemical processes**. The design of highly efficient solar-to-fuels generators that utilise water is both a formidable challenge and an opportunity that, if achieved, could have a revolutionary impact on our energy use system. Indeed, conventional renewables cannot yet accommodate large-scale generation of transportation fuel. One of the most promising avenues for the transformation of a current transportation economy lies in the discovery and harnessing of novel routes in the large-scale generation of renewable fuels.

1.3.3. Electrical storage

Lithium-ion batteries are currently the most efficient electrical storage solution in terms of energy and power densities. Their performances are incrementally progressing since their commercialization. Filling the gap between today’s performance and tomorrow’s energy demands requires step changes and emergence of new cost-effective and environmentally-safe concepts. These changes could arise from the development of new high-performance anodes, one of the current limiting factors. This will be a first focus in MOMENTOM.
Magnesium batteries are a longer-term attractive alternative, owing to magnesium natural abundance (low cost), high energy density (divalent ion) and lower reactivity (safety concerns). Their development is currently limited by the instability of standard electrolytes with Mg metal at low potentials. MOMENTOM will explore an innovative concept to solve this limiting issue by replacing the negative Mg metal electrode with a material compatible with electrolytes with wider electrochemical stability windows.
All-solid-state batteries are highly desirable for some mobile applications. They basically use an inorganic electrolyte with cationic conduction driven by mono and multivalent (Li^+, Mg^{2+} and Al^{3+}) ions to exchange the ions between the electrodes. This technology is safer than the Li-ion batteries, but requires the discovery of new **chemically stable and electrochemically efficient solid electrolytes** (with cationic conduction at ambient temperature close to 1 $mS.cm^{-1}$ and large electrochemical stability window).
Finally, supercapacitors are extremely interesting for many applications as they combine the high energy density of batteries with the high power density of double layer capacitors. High specific capacitance, excellent cyclability (more than 10.000 cycles without capacity loss) and low internal resistance are required. Nanostructuration is a strategy to achieve these goals since increasing the specific area leads to enhanced capacity and higher energy and power densities, while creating ionic pathways. It also allows for designing nanocomposites with another material of interest (metallic oxides, conjugated polymers). Synergetic effects are expected to give increased performances, provided the interfaces are smartly designed.

1.3.4. Socio-economic issues

One of the major challenges for future economies is the *transition* from brown energies (produced from polluting sources) to green energies (from renewable, non-polluting sources), the so-called **energy transition**. Hydrogen production is already a promising industry (about 80 million metric tons of hydrogen are produced with a yearly growth rate of 10%). However, this production remains dirty and costly: hydrogen is mainly produced from fossil sources (95%) and used in ammonia and hydrocracking processes. MOMENTOM addresses the questions of hydrogen and solar power as sources of green energy with a threefold interest. On the one hand, it considers fuel cells to convert chemical energy into electric power and vice-versa (storage). On the other hand, MOMENTOM develops new materials to convert solar power into solar fuels and to store more efficiently electrical energy. These research lines are complementary since finally solar power can be used to produce electric power and chemical energy. Such complementarity is crucial from an economic point of view: solar energy is already an integrated source in many countries but its intermittency represents a limit in terms of its proper integration in the system. The adoption of these new technologies corresponds to a cultural, sociological and political change.

The implementation of new technologies on a large scale to foster sustainable development requires policies embedded in an integrated strategy both at the macroeconomic level and at the industrial sector level. Due to the revolutionary properties of these new technologies, this implementation may contribute to significantly transform market segments and industries, develop new markets and stimulate economic growth both qualitatively and quantitatively (green and greening activities). We are particularly interested in the **transportation sector** (and mobility in general) in which technological and social innovation (materials, new energies platforms, smart grids, big data platforms and information and communication technologies) have become increasingly important with sustainability purposes (clean, safe, healthy and eco-efficient). Firstly, from the supply side, the implementation and use of these innovations are integrated into the supply chain contributing to higher value-added services. Secondly, from the demand side, the adoption and use of these innovations can also improve quality for users.

1.4. Objectives, originality and novelty of the project

The ultimate objective of MOMENTOM is to make the UPSay a recognised institution in the field of material research for energy by addressing some **ambitious challenges (capture, conversion, catalysis, storage)** that are crucial for the **energy transition** and by **taking into account also the economic and social issues** of these new energy technologies. The societal impact of this research is obvious, and it requires gathering expertise from chemists, physical chemists, physicists, and economists which makes Paris-Saclay an institution of choice for federating such a research. A strong added value is also to go beyond material research by studying the conditions of implementation of material advances. The economic aspects of these studies are part of the research performed in MOMENTOM, whereas aspects devoted to the resource and production managements will be performed in the parent project Grid4Earth. Therefore, together with Grid4Earth, MOMENTOM appears as a great opportunity to launch an integrated research on energy challenges at Paris-Saclay, with a critical mass which makes sense in the international competition.

MOMENTOM is also designed for triggering a joint effort dedicated to energy research and provides it with capabilities of maintaining and developing it after the end of the project. These development perspectives necessarily imply that the project should be relevant for the **long-term perspectives of industrial partners**, since the energy transition will actually be driven by companies which should provide efficient and cost-effective solutions to industrial and private sectors. For this purpose, the project is organised in two complementary mainstreams. The first one consists in working on selected targets during the running of MOMENTOM in order to obtain significant results relevant for the identified challenges. This way, MOMENTOM achievements should be a launching ramp for establishing joint teams or collaborative projects with industrial partners. In order to make this perspective realistic, the second mainstream of MOMENTOM is to set up a **Resource Center**. This original instrument will provide MOMENTOM teams a technical infrastructure favouring the running of their research projects, and also work for establishing links between MOMENTOM teams and industrial partners and favour information exchanges between the two worlds (what are industrial and economic needs, what are scientist skills and achievements).

Research actions within MOMENTOM have been chosen along three specific material **challenges** and one economic concern identified as instrumental for the energy transition: **hydrogen technologies, advanced**

solar energy, electrical energy storage, and quality vs. sustainability of the energy transition. Several topics have been chosen in each of these challenges and are described in the next part of the document. Parts of these topics are relatively mature, and correspond to pieces of solution for which significant results or proof of concept are reachable within MOMENTOM. Other parts are more prospective studies, less prone to immediate collaborative projects, but which have larger potential to yield technological breakthrough. Various instruments will be used for contributing the research projects, schematically post-docs for advancing more mature topics, master students for exploring more prospective projects.

The Resource Center will have a double purpose: a service role, and a contacting/communication role. The service role concerns both MOMENTOM teams and outside people or potential partners. For MOMENTOM teams, the Resource Center will provide assistance and expertise for developing scientific tools for dedicated material characterisation or lab-scale demonstrators through a shared prototyping platform. It will also propose to potential partners or individuals professional-oriented training programs concerning energy materials and systems. The Resource Center will also play an important role in advertising the activities, skills and results of MOMENTOM teams. A major aspect will be to establish relations between MOMENTOM teams and industrials in view of future partnerships or collaborations through various instruments described in the document. This will be assumed through the part-time enrolment of a specialist of industrial-scientific partnerships. The Resource Center will only organise a "matchmaking" between MOMENTOM teams and partners, on the basis of the team skills and partner needs, formal agreement remaining ruled by the parent organizations of the involved teams. Similarly, the Resource Center will be an instrument for the organisation of academic events with the purpose of both disseminating MOMENTOM results and establishing new consortia for future projects at the national and international levels. Finally, it will also organise outreach activities related to MOMENTOM projects, since energy transition is a process of primary societal concern interesting the widest audience.

2. Project organization, Scientific and technical program

2.1. Project management and structure

2.1.1. Management structure

The MOMENTOM project management and structure is described in **Figure 1**.

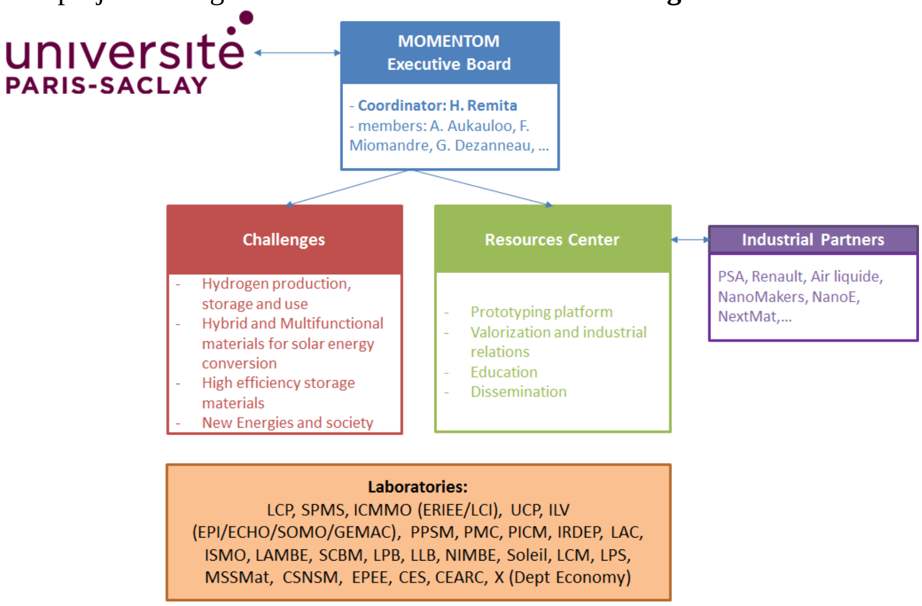

Figure 1. *Scheme of the MOMENTOM project organisation*

The project will be coordinated by **Dr. Hynd Remita** (see curriculum in **annex 3**) with the help of the Executive Board, whose role is first to represent the members of the consortium. H. Remita is Director of Research (DR1) at the CNRS. She is a physical chemist specialized in nanomaterials for photocatalysis and energy conversion. She has a large experience in team and research projects management.

The Executive Board consists of 11 members taken among the persons in charge of sub-WPs, namely: *DR. H. Remita (coordinator), Prof. A. Aukauloo (WP2.3), Prof. F. Miomandre (WP1.3), Dr. F. Ozanam (WP1.3), Dr. G. Dezanneau (WP1.1), Dr. J. Deschamps (WP1.1), Prof. E. Deleporte (WP1.2), Dr. W. Leibl (WP1.2),* *Prof. P. Schembri (WP1.4), Prof. P. Gaucher (WP2), and Dr. F. Plais (WP2.2).*[8] The Executive Board is also the body in charge of the implementation and monitoring of the project. Its role is thus to take all decisions necessary for the implementation of the work-program and to report to the University Paris-Saclay.

2.1.2. Meetings/reporting

The Executive board will elaborate detailed implementation plan for the project after the kick-off meeting. Throughout the duration of the project, it will hold at least 4 meetings per year and will make the object of a meeting report distributed to all members of consortium via the **intranet network**. The purpose of this EB meetings is to take operational decision concerning the budget, the organisation of events, the deadlines for reporting…The EB will also collect and maintain the deliverables.
Annual reports will be provided as a basis of discussion for annual meetings. These meetings will concern both scientific and management aspects. Typically a 2-day meeting will include a first day for scientific presentations, a second day will be more dedicated to management and organization aspects, such as non-permanent staff venues and exchanges, budget state, scheduled participation to conferences, workshop organization…Non-permanent staff will be encouraged to present their results during annual meetings.

2.1.3. Project organisation

The project will be declined in 2 parts that will represent 2 Work Packages (see **Figure 2**):
- **WP1: Challenges:** The object of this work Package will be the exploration of challenges in the field of materials for energy and associated economic aspects. We chose to focus on specific energy challenges related to the expertise of the involved laboratories and for which the MOMENTOM project allows reaching the critical mass of researches to expect significant breakthroughs.
- **WP2. Resource Center:** The object of this WP is to develop a specific entity within the MOMENTOM project to settle the conditions of sustained industrial relations. Concretely, the Resource Center will help the laboratories to build lab-scale demonstrators, and prototypes for *in-operando* characterisation, will valorise the scientific advances obtained at the European level, will promote industrial relations by favouring exchanges with identified partners. Professional education, training actions and workshops are also foreseen within this WP as well as dissemination actions toward the large public.

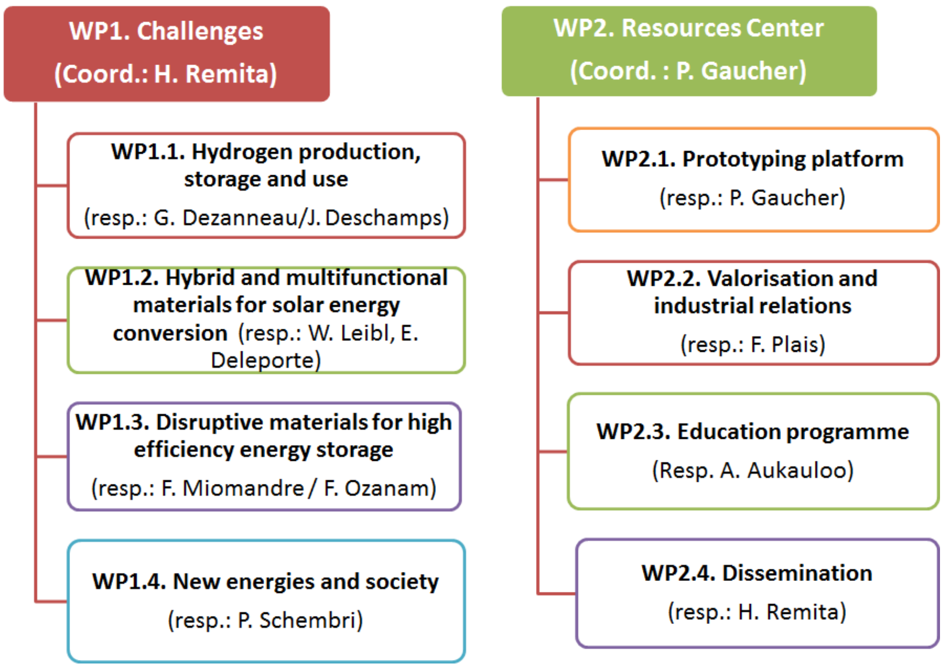

Figure 2. *Scheme of the MOMENTOM work packages*

2.2. WP1 - Challenges

As defined above, we have chosen to focus our research efforts on specific challenges, more specifically on hydrogen technologies, on solar energy conversion into chemical energy, on electrical storage, and on social/economical aspects around these new energy technologies. The first market of these technologies would essentially concern transport/mobile applications, but other important markets are also concerned such

[8] Details on the executive board are in annex 4.

as the one of industrial hydrogen. The list of the laboratories involved in each challenge with the number of researchers involved (including the men/months) is given in **annex 4**.

2.2.1. Hydrogen production, use and storage (WP1.1.)
Resp.: G. Dezanneau (CNRS/CentraleSupelec), J. Deschamps (ENSTA)
11 Laboratories involved, 46 researchers

As mentioned previously, several challenges remain for facilitating the deployment of hydrogen technologies. For low temperature electrolysis and fuel cells, the main current limitations are the production cost mostly due to precious metal catalysts, and the limited lifetime. For high temperature fuel and electrolysis cells, lifetime is also an important issue, which can be overcome by developing new Solid Oxide Cells working at lower temperature for instance based on proton conductors. The hydrogen storage also represents a crucial problem, especially for mobility and on-board applications. Currently, only two on-board storage techniques are available: the liquid state storage at very low temperature (20 K) and the storage under high pressure (700 bar). An alternative solution for hydrogen storage at moderate temperature and pressure has to be developed. MOMENTOM will address all these limitations through targeted topics aimed at promoting the development of hydrogen as a future energy carrier through innovative solutions and efforts to understand the underlying physical phenomena.

<u>**Low temperature electrolysis and fuel cells**</u>

The large-scale deployment of PEM-based electrolysers requires **the development of low-cost and precious metal-free catalysts,** using advances in the transition metal molecular chemistry or hybrid materials. This development should be performed together with the implementation and test of innovative solutions in high power prototypes, in relation with industrial partners. MOMENTOM will focus on the following topics.

Topic 1. New precious metal free electrocatalysts. MOMENTOM partners aim at pursuing their effort in the implementation of new electrocatalysts based on molecular chemistry, either in solutions or adsorbed on electrodes such as metallic oximes, clathrochelates, thiometallates, polyoxometallates, but also metallic nano-objects, or carbon-based nano-objects, or nanostructured conducting/semiconducting materials on high specific surface electrode materials. The electrocatalysts should allow for (i) operation at low (0-100°C) temperature; (ii) use of strongly acidic polymer electrolytes; (iii) dense packing for operation at elevated current densities (several $A.cm^{-2}$) and high conversion efficiency (> 75%). Molecular chemistry of transition metals offers fascinating alternative opportunities to nano-platinum group metal electrocatalysts, to prepare reaction-customized (photo)-electrochemically active interfaces: (i) possibility to perform electrocatalysis at molecular scales; (ii) high versatility: possibility to design tailored electrochemical nano-reactors using mono-/poly-nuclear complexes of appropriate chemical composition, geometry and activity; (iii) functionalisation of nano-structured catalysts on either 2D or 3D electrodes made of conducting (glassy carbon, carbon fibrous, nanotubes, graphene) or semi-conducting materials (TiO_2, $SrTiO_3$, $BiVO_4$, NiO…). Within MOMENTOM, the efficiency and robustness of these new 2D and 3D interfaces obtained by chimisorption or physisorption of complex molecular catalysts (see **Figure 3**) will be improved.

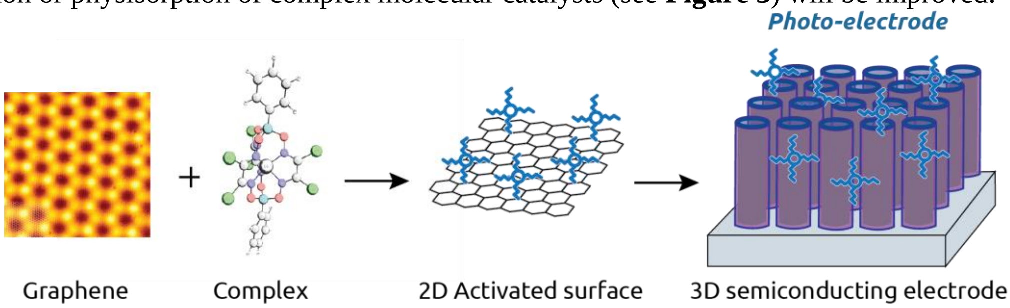

Figure 3. *From 2D towards 3D activated electrodes by functionalization of molecular catalysts.*

Innovative techniques will be developed for the synthesis and characterisation of densely packed (to take advantage of the entire surface of carriers) and topological-oriented (to enhance electro-activity) molecular structures at molecular level. A special attention will be paid to the influence of the auto-assembly parameters varied during the ink preparation on the final electrocatalytic properties when deposited on model substrates. Efficient catalysts without (or with a small amount of) noble metals will be synthesised, and the existence of synergetic effects between catalysts on the one hand, and between the catalyst and the host substrate serving as electrode will be investigated.

Topic 2. Reversible fuel-cell mode/electrolyser mode systems. In the design of a regenerative fuel cell, two approaches may be taken: (i) the fuel cell and electrolysis units may be kept separate; (ii) only one unit operates as a fuel cell and an electrolyser, in other words, as a "unitised" regenerative fuel cell. MOMENTOM will develop efficient PEM unitized regenerative fuel cells (PEM-URFCs) with platinum free or very low platinum-group-metal loadings and improved lifetime performances during cycling. The key technology in the development of the unitised regenerative fuel cell is a bifunctional catalyst and electrode able to operate in both the fuel-cell mode and the electrolyser mode.

High temperature Proton-Conducting Fuel and Electrolysis Cells.

Proton conducting Fuel or Electrolysis Cells (PCFCs / PCECs) now emerge as a robust alternative to SOFCs/SOECs. Their main interest lies in an operation at intermediate temperature *i.e.* around 500°C. In this case, the durability of the device is expected to be much higher and the applicability can be extended more easily to mobile applications for which fast turning-on of the device is needed. **PCFCs can achieve excellent performance (455 mW.cm^{-2} at 500 °C) and long-term durability (>1000 hours without loss)**[9]. In spite of these promising and impressive results, questions remain about the scaling-up of the process and the durability of $BaZr_{1-x-y}Ce_xY_yO_{3-d}$-based fuel cells in stack conditions. Understanding the elementary reactions in these proton-conductor devices and improving their efficiency are still needed. MOMENTOM will focus on the following topics:

Topic 3. Development of specific electrode materials with mixed proton-electron conduction: until now, good air electrode materials (anion-electron conductors) have been used in PCFCs, so that electrodes represent 20-30% of the cell resistance at 500 °C. Then, possible progresses lie in the development of proton-electron conductor materials. Promising results have been obtained for $BaCo_{0.4}Fe_{0.4}Zr_{0.1}Y_{0.1}O_{3-d}$ whose excellent properties seem to be due to proton incorporation and diffusion. Further developments are needed to quantify the contribution of proton in the air electrode mechanisms, using combined advanced experimental methods (nuclear microprobe[10], conductivity relaxation[11]) and DFT theoretical calculations[12].

Topic 4. Explore the durability and aging mechanisms in PCFCs and in PCECs: while Solid Oxide Fuel Cells have been tested at high temperature for long periods (typically 30000-50000 h), similar tests have not been performed yet for Proton Conducting Fuel/Electrolysis Cells. A deeper understanding of the aging mechanism in PCFCs/PCECs is thus needed. MOMENTOM will perform long term tests and analyse the evolution of both electrolyte and electrode materials, and of their interfaces, with specific attention to the influence of water pressure on electrode material degradation and to the inter-diffusion of species at the electrolyte-electrode interface. Local hydrogen concentration will be measured at a micrometer scale using Ion Beam Analysis (IBA) which will be combined with STEM analysis for performing chemical maps with atomic-scale resolution and FIB 3D reconstruction to quantify the evolution of the electrode components.

Hydrogen storage

MOMENTOM will focus on solid state storage by adsorption in porous materials, which appears as a promising and efficient alternative solution for hydrogen storage at moderate temperature and pressure**.**

Topic 5. Hydrogen Storage at low pressure in meso(nanoporous)materials

Metal-organic frameworks (MOFs) are crystalline porous materials consisting of metal ions or metal clusters and organic ligands as linkers. MOFs possess very low densities, huge surface area values, adjustable pore size and functionalising ability of pore walls. However high hydrogen uptake capacities reported in MOFs were at cryogenic temperatures only. Doping of MOFs with various carbonaceous yielded a composite with unusual mechanical and hydrophobic properties and enhanced adsorption capacity (× 1.5 at ambient temperature under 100 bar).[13,14] Recently, ENSTA ParisTech developed post synthetic methods of metal doping of activated carbon-MOF composites, and preliminary results showed extended hydrogen storage

[9] C. Duan, J. Tong, M. Shang, S. Nikodemski, M. Sanders, S. Ricote, A. Almansoori, R. O'Hayre, *Science*, 349, 1321-1326, 2015
[10] S. Sorieul, S. Miro, M. Taillades-Jacquin, J. Dailly, F. Mauvy, M.-H. Berger, and **P. Berger**, Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, vol. 266, no. 8, pp. 1430 – 1433, 2008.
[11] P.-M. Geffroy, Y. Hu, A. Vivet, T. Chartier, **G. Dezanneau**, *J. Electrochemical Society*, 161, F153-F160, 2014
[12] G. Geneste, A. Ottochian, J. Hermet, **G. Dezanneau**, *Phys. Chem. Chem. Phys.*, 17(29), 19104-19118, 2015
[13] Prasanth K. P. and **Deschamps J.**, *Journal of Material Chemistry A*, 3, **2015**, 7014.
[14] Prasanth K. P. and **Deschamps J.**, *Journal of Porous Materials*, 22, **2015**, 1635.

capacity of a material (×4 at ambient temperature under 100 bar).[15] MOMENTOM will extend the variety of MOF composites by using different forms of carbon and developing new metal-doped composites by post synthetic treatments of the MOF composites. Porous metal nanostructures such as palladium nano urchins[16] and 3D-porous nanoballs (Pd-Pt, Pd-Ni, Pd-Co),[17] developed at LCP, will be tested. Efficient bimetallic porous nanostructures with a low amount of precious metal (Pd) will be also developed to decrease the cost.

2.2.2. Hybrid and multifunctional materials for solar energy conversion (WP1.2.)

Resp.: Dr. W. Leibl, E. Deleporte (CEA/ENS Cachan)

19 Laboratories involved, **60 researchers**

In order to optimise the conversion and storage of solar energy, different research groups of the UPSay will join their expertise to **integrate photoactive cells and electrolyser functions** for the production of **solar hydrogen fuel**. The project will gather the expertise, know-how and large variety of analytical techniques existing at the participating institutes to achieve breakthrough in the field of photoelectrochemical cell technology. The strategy pursued is to obtain multifunctional materials by coupling basic elements developed by the different partners with particular attention to the control of interfaces in the hybrid assemblies and to protection against photocorrosion, which are crucial for efficiency and stability[18].

Within this workpackage, two kinds of devices will be developed:

- **Photovoltaic-aided electrolysers:** with this device (see **Figure 4**), a photo-induced voltage will be used to obtain the desired electrolysis reaction. Two types of photovoltaic sub-components will be developed, derived from a silicon-based technology, the other one from the recently discovered hybrid perovskite materials. This original device will be treated in topics 6-8.

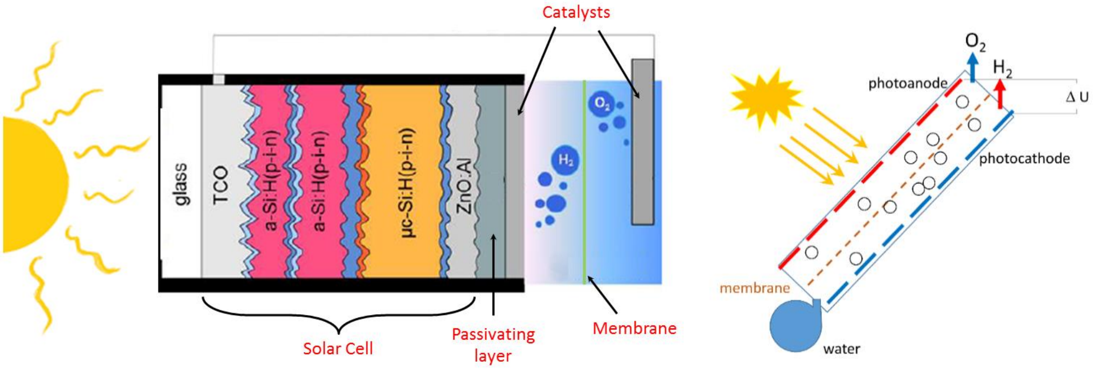

Figure 4: *Schematic representation of a photoelectrochemical device developed in the project*

- **Photo-assisted PEM electrolysers:** In this device, a classical PEM will be reinvented so as to include a photo-catalysis reaction. It is expected that the electrolysis reaction will be obtained at a higher rate or lower voltage. It will be treated in topic 9.

Topic 6. Development of modified SiNW based photoelectrodes

The objective is the development of photoelectrolysers based on Si-nanowires (SiNW) photoelectrodes incorporating appropriate passivation layers. Very few examples exist where multi-junction Si electrodes have been used to develop hybrid photoelectrodes for the water oxidation reaction or the reduction of CO_2 in solution.[19] SiNW have also been used for the deposition of metal oxide catalysts for the oxidation reaction[20]. SiNW devices have proven promising for high performance and high surface solar cells[21]. Low-temperature deposition as well as plasma-enhanced vapor-liquid-solid nanowire growth assisted by inexpensive Sn make SiNW devices good candidates for our state of the art PEC cells. The nanowire devices feature the following interesting properties for the targeted application:[22,23,24,25]

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[23] Kelzenberg, M. D.; Boettcher, S. W.; Petykiewicz, J. A.; Turner-Evans, D. B.; Putnam, et al. *Nature Materials* **2010**, *9*, 368

- Low cost due to a low-temperature production process;
- Very strong light trapping due to the optical properties of nanowires;
- Very high surface to volume ratio;
- High open-circuit voltage (V_{oc}) up to 0.9 V for single junction and >1.5 V for radial tandem device.

The last two properties, normally competing in classical PV devices, are achieved simultaneously due to a very efficient surface passivation during the radial junction solar cell fabrication. By designing triple radial junction devices, V_{oc} over 2 V can be expected. The fabrication of these devices is based on established procedures at LPICM based on plasma-assisted vapor-liquid-solid growth of nanowires. The growth will be adapted to metallic substrates to allow easy electrical connection for the use in the PEC. Planar devices (1 to 20 cm^2) will be first fabricated to provide partners with test devices to start developing steps necessary to assemble all building blocks. High V_{oc} (>2 V) devices will be fabricated using hydrogenated amorphous, polymorphous, and microcrystalline silicon absorbers in double or triple junction configurations.

Passivation layers will serve as templates for deposition (resp. attachment) of metal oxide (resp. molecular) catalysts. The most obvious candidates for conductive passivating materials needed for PEC cells are n-type Si-oxide layers developed by PICM. Alternatively, different interfacial layers (TiO_2 and C nanostructures) were recently developed by the NIMBE laboratory to improve the charge transfer between an organic cell and a MoS_2 catalyst for hydrogen photo-production[26]. Ti interfacial layers have been used to drastically increase the photocurrent. The efficiency of these layers will be assessed, together with polyphosphazene (ILV) passivation[27] on (-*n* and –*p*) InP[28] or He-ion irradiation at moderate energy and fluences (CSNSM).

Topic 7. Development of photoelectrodes based on hybrid perovskites

Similarly to SiNW-based devices, photoactive devices based on hybrid perovskites are very promising for the generation of electrical power due to their high photovoltaic performances.[29] They have been successfully used for light-driven water splitting, but the perovskite instability limited the cell lifetime.[30] The study of the different sources of instability is an intense research field. Another key topic concerns the interfaces of the hybrid perovskites with the other intra-device layers (electron or hole transporting layers).

A first objective is to **understand the mechanisms governing the phase properties** in addressing the phenomenon at the stage of $CH_3NH_3PbI_3$ type perovskite synthesis by the analysis of structural, physical and optical properties. The bulk and surfaces/interfaces properties will be revealed by X-diffraction and photoemission (LPS), XPS, Auger spectroscopy, and SEM-EDS (ILV, GEMAC). Optical experiments such as continuous and time-resolved photoluminescence (LAC), cathodoluminescence (ILV/GEMAC), FTIR, Raman spectroscopy will allow elucidating the excitonic and vibrational properties and will give insight into the nature of the defects inside the thin layers. THz spectroscopy and Time-Resolved Microwave Conductivity (LCP) will for allow measuring the dynamics of charge carriers.

A second objective is to **modify and control the hybrid perovskite itself and its interface** with other layers: such modifications will allow for better understanding and seek for **increasing the stability,** e.g., at the perovskite / substrate interface: ILV and LPICM will work on the controlled perturbation of the absorbing material, alone and integrated in the device by setting up a methodology of controlled genesis of the degradation and a metrology analysis combining chemical, electrical and optical approaches. A great advantage of the hybrid perovskites is their flexibility, i.e. the possibility of molecular engineering on both the organic and inorganic parts of the molecule (LAC, PPSM). He-ion irradiation (CSNSM) will be used for controlled defect engineering and adjusting the doping level to tune carrier concentrations.

Topic 8. Deposition of catalysts for the photo-dissociation of water, building and tests of complete cells

N**ew catalysts** will be deposited on the photoelectrodes for **water oxidation** and **proton reduction,** with the central idea to replace noble metal catalysts by cheaper, but similarly efficient and stable systems. Molecular manganese and iron complexes as investigated at ICMMO and LPB[31] are good candidates for catalysts for

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[29] see NREL chart gathering efficiencies of solar cells, http://www.nrel.gov/ncpv/images/efficiency_chart.jpg
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water oxidation and will be covalently grafted to the photoanodes. For the photocathode, we will use the novel cobalt-based molecular catalysts for H_2 evolution that have been shown to lead, upon reduction in presence of acids, to the formation of highly active cobalt **nanoparticles** (electrodeposition or radiolytic reduction)[32]. Radiolysis allows also synthesis bi- or multimetallic nanoparticles (based on Ni, Co, Fe, etc).[33]

Metal oxides catalysts based on cobalt, iron or Mn that have previously shown catalytic properties toward water splitting in highly acidic conditions will be studied at higher pH. The aim is to have an efficient catalyst that works at the same pH than the catalyst at the (photo)cathode. The targeted pH range is between 3 and 4. For easy deposition the catalysts should be made by sol-gel process, hydrothermal technique or radiolysis. Thus the cobalt phosphate catalyst that has recently been reported by some of us to split water in acidic and neutral medium, will be used at the photo-anode. A new synthesis method will be developed to obtain solutions of cobalt phosphate nanoparticles processable by spin- or spray coating.

Molybdenum sulfide is a very efficient catalyst for proton reduction, but only in highly acidic conditions (0.5 M in sulfuric acid). To improve the chemical stability of photocathodes alternative inorganic catalysts based on Mo, Co, Cu, Ni, or W will be studied to work at higher pH. Thus, recently reported electro-catalysts like ternary sulfide of (Cu_2MoS_4)[34] or of cobalt–tungsten and nickel–tungsten[3516] which present efficient and robust electrocatalytic properties for the HER in water over a wide pH range will be synthesized in nanoparticle form to be spray-coated or spin-coated on different electrodes.

For the characterisation of the hybrid materials developed in **topics 7 and 8**, and the development of a functional PEC cells, different characterisation techniques will be used (p.16). We will study the reaction sequences occurring after light excitation and to identify bottlenecks and degradation pathways.

This topic finally includes the testing of these photoelectrodes in well characterized half-cells and their coupling in a PEC prototype device. For the construction of a **complete PEC device** two architectures will be tested: a single high-performance photoanode coupled to a cathode or photoanodes and photocathodes in a tandem configuration. In the latter case, light excitation of the two electrodes has to be managed by adjusting the absorption properties or geometrical architecture. The best photocathodes and photo-anodes will be assembled with a proton-conducting membrane to make the target device. Small-scale test cells are available for example at LPB, larger versions will be developed at the prototyping platform.

Topic 9: Photo-assisted PEM electrolyser.

Parallel to the photovoltaic-aided electrolyser, we will develop an innovative concept of hybrid photo-electrochemical cell for the photo-assisted electro-dissociation of water and the production of hydrogen of electrolytic grade. The concept is that of a PEM (polymer electrolyte) cell equipped with two photo-electrodes that will perform the endergonic water dissociation with an input of both photons (sunlight energy) and conventional electricity, the proportion of which being an operating parameter, adjusted as a function of sunlight availability .

It aims at providing a photo-assistance to a conventional water electrolysis cell that has poorly been considered in academic research. Differently put, if one or two photo-electrodes are incorporated to a PEM water electrolysis cell, it can be expected that absorption of sunlight radiation will alleviate the electricity consumption (in kWh/kg H_2) required by the DC power source alone. The main goal will be first to develop and test efficient photoanodes and photocathodes active in acidic aqueous media, then to incorporate them in the PEM water electrolysis cell. Practical developments will be limited to the monocell up to 250 cm^2 and tests will be performed using sunlight simulators available within the consortium. To reach this goal, MOMENTOM consortium will offer the inputs of experts on semiconductors, molecular electrocatalysis and electrochemical engineering.

2.2.3. Disruptive materials for high efficiency energy storage (WP1.3.)

Resp.: F. Miomandre (ENS Cachan) / F. Ozanam (CNRS/Ecole Polytechnique)

11 laboratories involved, 32 researchers

[32] Cobo, S.; Heidkamp, J.; Jacques, P.-A.; Fize, J.; Fourmond, V.; Guetaz, L.; **Jousselme, B**.; Salazar, R.; Ivanova, V.; Dau, H.; **Palacin, S**.; Fontecave, M.; Artero, V. *Nature Materials* **2012**, *11*, 802.

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MOMENTOM will develop innovative systems and materials for electrical storage (batteries and supercapacitors) of potential industrial interest in the coming years. The project will focus both on the synthesis of materials and on the fundamental understanding of the phenomena at work in the devices through advanced characterisation. The coupling between synthesis and characterisation will facilitate strong collaboration between the different partners and open the way to ambitious national and European projects around MOMENTOM. As sketched in **Figure 5**, four different research axes, with different degree of maturity (from high to low) will be considered.

Topic 10. Advanced Li-ion: high energy density and efficient anodes. Silicon based negative electrodes could theoretically increase the energy density of the negative electrode of Li-ion cells by a factor of 10 as compared to graphite currently used in commercial batteries, but are not yet developed at the industrial scale due to rapid fading of the performance. In order to overcome this issue, MOMENTOM will focus on two innovative systems: core@shell Si@C nanoparticles and Si-methyl thin films. These two electrode materials have been elaborated within MOMENTOM teams and present promising characteristics for improving the electrode stability. A new class of hybrid materials, polyoxometallate (POM)-carbon composites, will also be investigated. Due to the high number of electrons that POM compounds exchange during oxidation/reduction process (more than 10 with some specific metallic centers), they could advantageously increase the energy density of the battery. MOMENTOM teams have a recognized expertise in these materials (both in terms of syntheses and electrocatalytic properties) and thus are best suited for assessing their inedited use as active materials for high power secondary batteries. For all of the selected systems, a combination of techniques (TEM, XPS, X-Ray analysis, FTIR, nuclear probe) will be used, possibly coupled to advanced electrochemical characterisation such as impedance spectroscopy for better understanding the elementary electrochemical processes occurring from the interface to the bulk of the electrode.[36] This effort is aimed at assessing the performances of the materials and architectures in the conditions of battery operation.

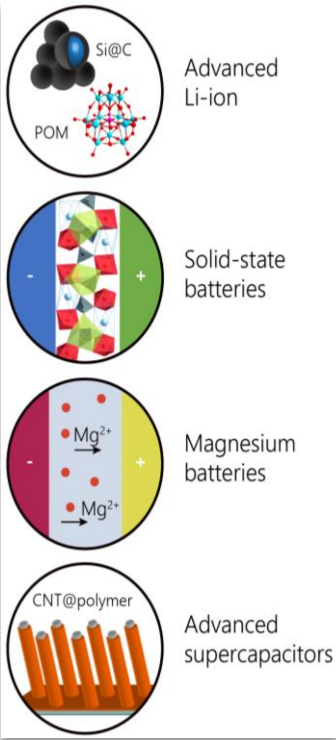

Figure 5: *the four topics of the challenge "Disruptive materials for high-efficiency energy storage"*

Topic 11. Solid-state batteries. All-solid-state batteries using an inorganic electrolyte with cationic conduction driven by mono or multivalent (Li^+, Mg^{2+} and Al^{3+}) ions is another technology favored by industrials, since it can provide high energy density and solve safety problems. MOMENTOM teams will synthesize new solid electrolyte materials (Garnet and Nasicon-type materials and new high entropy oxides[37] exhibiting superionic conductivities at room temperature) and optimise the assembly conditions with electrode materials. Combination of electrochemical characterisation, structural, spectroscopic and analytical techniques available in the MOMENTOM consortium will deepen the understanding of the cationic dynamics (mono and multivalent) through structured networks of the material. Of great interest is the study of the interfaces between the solid electrolyte and the electrode, poorly studied in the literature while it will be the main hurdle to overcome to envision a commercialisation. This is precisely a domain in which MOMENTOM teams have recognised expertise and can access a set of relevant characterisation techniques.

Topic 12. Magnesium-ion batteries: high energy and stable anodes. Mg batteries using Mg metal as negative electrode show great promise as a high energy, cost-effective and safe battery technology. However, magnesium metal is not stable in conventional electrolyte solutions, preventing its use in the battery. On the contrary, Mg alloys compounds, analogous to the Li alloys negative electrodes, possess adequate stability in conventional electrolytes and slightly higher potentials than pure Mg metal. MOMENTOM teams will then elaborate **high capacity and efficient negative electrodes**, based on nanostructured Mg alloys compounds. Unexplored binary or ternary alloys (based on Mg with Sn, Sb, Bi, In, Ga) will be synthesised in order to obtain cycling performance (capacity, coulombic efficiency) higher than the state-of-art materials. The

[36] S. Larfaillou, D. Guy-Bouyssou, F. Le Cras, S. Franger, J. Power Sources 319, 2016, 139
[37] D. Berardan, S. Franger, A.K. Meena, N. Dragoe, J Mater Chem A 4, 2016, 9536

nanostructuration will be beneficial to develop highly efficient negative electrodes for Mg-ion batteries, mitigating the large volume changes predicted upon full magnesiation and enhancing the sluggish diffusion of Mg^{2+} ions in the solid. Here again, electrochemical and structural/morphological characterizations will be used for understanding of the magnesiation/demagnesiation reaction mechanisms of the new compounds. A particular attention will also be paid on the reactivity at the interface of the electrode with the electrolyte.

Topic 13. Advanced nanostructured materials for supercapacitors. Carbon nanotubes (CNT) are good candidates as electrode materials for supercapacitors due to their high specific area, especially when designed as aligned carpets according to a CVD process now well mastered in the CEA/NIMBE group. In that case they can host a secondary active material like a conducting polymer or metal oxide nanoparticles leading to very high capacitance values when ionic liquids are used as the electrolytes.[38] For optimizing these assemblies, the initial formation of metallic oxides on the CNT surface will be first investigated *ex-situ* using X-ray absorption and fluorescence spectroscopies to make further correlation with the morphological and structural analysis of the active material upon electrochemical solicitations obtained by *in operando* analysis. Other materials will be considered. CNTs will be associated to PVDF to get CNT/PVDF binary composites and boron nitride nanosheet (BNNS)/CNTs/PVDF ternary composites with different molar ratios. We will use the combination of solution casting and extrusion-injection processing in order to achieve an optimal dispersion of nanofillers in the PVDF matrix. Functionalised graphene sheets modified through covalent linkage are also promising materials since the decrease of the intersheet interactions can be used to insert other energy storage materials like conducting polymers to design highly capacitive hybrid materials as shown in PPSM.[39] Finally, new high entropy oxides, recently synthesized,[40] exhibit huge dielectric permittivity on a wide frequency domain, and its value can be tuned by the temperature and/or the chemical composition, which can be of great interest for supercapacitance applications.

2.2.4. New energies and society (WP1.4.)

Resp.: P. Schembri (UVSQ)

4 laboratories involved, 11 researchers

MOMENTOM will tackle the new energy issues from a macro and microeconomic perspective. A theoretical model will formalise the **regime switching** from brown **to green technologies**, and, starting from available empirical data on hydrogen and solar power, we will simulate future scenarios considering alternative public policies to implement the regime switching. After considering the economic transition at the macro level, we the micro level will be used through a **sector analysis**, studying the impacts of the investment strategies (in green technologies) in the electric/mobility sector (uses, analysis of supply and demand, innovation adoption). This research will be complemented by a **field study** on land transportation to test the relevance of our research program, bridging the macro-micro and normative issues and contributing to their relevance.

Topic 14: Energy transition (macroeconomic approach). The energy transition will be modeled with sustainable growth models with **regime switching** (dynamic general equilibrium models coupling traditional endogenous growth literature with technological change and (non-) renewable resource and pollution models mainly used in environmental economics). The difficulty is on the computation of explicit analytical trajectories including the switching and the tipping point so as to provide robust conclusions. From a mathematical point of view, the existence of solutions will be addressed through standard topological arguments, while the stability properties, including the technological switching, will be analysed through the bifurcation theory (either local or global). From an economic point of view, we will compare the first best (planner's solution facing resource constraints) with the second best (market solution based on prices under public policies (fiscal policy and pollution permits). The first best takes into account not only the production but also the pollution level and their impact on future generations. The optimal trajectory is characterised by two successive regimes: first, the economy uses the fossil resources, pollutes and finances the R&D on green technologies, and then it adopts these new technologies based on the **complementarity between renewable energies and hydrogen**. The way to discount the future and weight the welfare of future generations remains a controversial issue that will also be discussed. The introduction of (energy) policies makes the positive model more difficult to solve. Starting from available empirical data on hydrogen and solar power, we will

[38] S. Lagoutte, M. Pinault, P-H Aubert, F. Tran-Van, C. Chevrot, D. Sarrazin; FR2962450, WO 2012/004317 A1 ; S. Lagoutte, P.H. Aubert, M. Pinault, T.V. Francois, M. Mayne-L'Hermite, C. Chevrot, Electrochim. Acta, 130, 2014, 754.
[39] Li Y., G. Louarn, P.H. Aubert, V. Alain-Rizzo, L. Galmiche, P. Audebert, **F. Miomandre**, Carbon 105 (2016) 510-520
[40] D. Berardan, **S. Franger**, D. Dragoe, A.K. Meena, N. Dragoe, Phys Status Solidi RRL **10**, 2016, 328

simulate future scenarios according to alternative public policies to promote regime switching and we will provide **policy recommendations**. The numerical simulation of future scenarios has to take into account the energetic transition to hydrogen and solar power based on (public) investments in R&D and on other policy solutions identified in the theoretical model). The very question remains how to finance the energy transition either on the supply side (R&D and infrastructures) or on the demand side (education and communication to change individual and social preferences). Traditional policy tools such as taxes or subsides could turn to be inappropriate in the current globalized context where externalities, free-riding and public budget constraints play a role. Other solutions based on new financial engineering and leverage jointly with the restorations of missing markets (pollution permits) may represent suitable alternative to a traditional fiscal approach. Anyway, the issue remains to estimate whether empowered fuel cells and new nanomaterial to convert solar power will significantly impact economic growth and reduce emissions causing global warming or will remain an epiphenomenon even in presence of proactive public policies.

Topic 15: Mobility (multi-sector analysis and field study). Macroeconomic representation is suitable to capture economic transitions/bifurcations. However, a multi-sector analysis is necessary to capture the complementarity between hydrogen and new energies. Dynamic general equilibrium models are more complicate to handle sector-specific aspects. To capture the integrated energy-mobility system, we will develop an input-output model extended to include electro-mobility and its environmental implications (**sector analysis**). We focus on investment strategies and the corresponding impacts of investments on society. The relationship between the costs and benefits of these new energies and the scale and profile of investments will be assessed. We study the extent to which the technological solutions need to be applied and involve up-front capital investments, as well as the subsequent lifespan of the corresponding assets. We focus on the speed at which they can be deployed by using a neo-Schumpeterian approach of technological change based upon the notion of path dependence. With respect to the temporal dimension of sustainability, we examine the extent to which current investment strategies facilitates (or limits) the ability of the system to adjust investment strategies in response to new information about the value of these technological solutions in the mobility sector. **Land transportation** (passenger and merchandise) is a major and growing segment of GHG emissions. It is also responsible for local and regional pollution going along with the increasing urbanization. Hydrogen can play a significant role in the decarbonisation of land transportation. This sector provides a major opportunity for deepening and testing our research. Firstly technological innovation in hydrogen has to be analyzed in a context of parallel developments in other technologies such as electric battery; Green and efficient production and storage of hydrogen are keys in this technological race. Secondly, changes in behavioral habits play an important role in reshaping the various modes of transportation (private versus collective, car sharing…); These changes have to be integrated in future demand trends. Thirdly, multiple policy instruments are commonly used to promote green technologies in transportation both upstream (R&D, infrastructures) and downstream (rebates on vehicle purchasing price as well as various perks such as access to express lines or free parking); The efficiency and consistency of these instruments remain problematic. This **field study** will allow for building bridges between the macro-micro and normative issues addressed in this research program and contribute to their relevance.

2.2.5. Implementation of WP1: Challenges

Research actions

WP1 is dedicated to the exploration of research challenges, which will make the object of significant efforts by the involved laboratories (more than 688 men.month all along the project corresponding to 19 full time equivalent (FTE)). Specific actions will be launched by MOMENTOM to facilitate the realisation and building of inter-laboratories projects: Master students, post-docs… We expect also that ANR projects will be launched during the generic call of 2017, involving several groups of the MOMENTOM project. As such, the joint reflexion necessary for the building of the MOMENTOM project has been particularly useful for generating new ideas and innovative research paths.

Young researchers recruitment

We have identified **15** strategical topics to be explored within the MOMENTOM project. In support to the proposed research orientations, we ask for some budget to recruit post-doctoral researchers. These will be recruited exclusively on one of these **15** topics. The selection of the candidates will be realised by the Executive Board on the following criteria: excellence of candidate, inter-laboratory character of the proposed

research, novelty and impact of the post-doc project. In the **phase 1** of the project (asked by University Paris-Saclay), and in order to start quickly on the topics considered as strategically the most important, we have chosen to fund four 1-year **post-doctoral positions** on the following topics:
- New platinum-free electrocatalysts for Proton Exchange Membranes (WP1.1., Topic 1)
- Photoelectrodes for the chemical conversion based on Silicon nanowires (WP1.2., Topic 6)
- Anodes materials for efficient electrical storage (WP1.3., Topic 10)
- Energy transition, economic policy, land transportation (WP1.4., Topic 15)

For the **Phase 2**, a call will be launched at the end of 2017 to recruit a second batch of 7 post-docs for 1-year contracts to start at the very beginning of 2018.
For the attribution of **master grants**, there will be also a 2-phases process. For **phase 1**, the executive board will attribute these master grants on topics not covered by post-docs. These master grants will allow selecting and preparing good PhD candidates f. A similar process will be launched for the **phase 2**, by the end of 2017.

Specific instrumentation for characterising the materials

The Paris-Saclay University (UPSay) gathers a unique ensemble of characterisation methods and tools that can be used in order to describe and optimise the energy harvesting and conversion systems developed within this project. State-of-the-art facilities encompass, e.g., bulk structural properties (XRD, Raman spectroscopy, …), surface characterisation (XPS, Auger, …), electrical and electrochemical measurements, (cyclic voltammetry, impedance spectroscopy in working conditions, chronoamperometry, dielectric measurements, breakdown voltage, …), catalytic, electro-catalytic and photocatalytic properties, nanoscale chemical characterisation (STEM, SEM, NanoIR….). More dedicated available techniques include **Tera Hertz spectroscopy** and **Time resolved Microwave conductivity** (TRMC) to study the charge carrier dynamics respectively at fs/ps and ns time scales and **time-resolved optical and photocurrent measurements** to obtain further information on the **dynamic properties.**
"In-Operando analysis" refers to non-destructive techniques used to follow the physicochemical processes occurring in a device during its operations. The aim is to analyse how the interaction between different components affects the efficiency of the device as well as its aging. Reaction products (O_2, H_2) will be quantitatively determined by GC/MS to determine Faradaic yields. Together with quantification of the incident photon flux, this will determine overall energy conversion yields for the devices. Stability will be assessed by measuring the current over extended time periods. For in operando characterisation, specific sample holders will be developed at the prototyping platform within the MOMENTOM Resource Center.
Among others, **the nuclear microprobe analysis** can be used to probe a sample with energetically light ion beams (protons, deuterons, helions-3 and helions-4) and analyse the material composition through the interactions generated with the atoms encountered on the pathway. These measurements can be performed *ex situ* and now *in situ/in operando* thanks to the development of an electrochemical cell dedicated to nuclear probe analysis (patent in preparation). This technique has already been successfully applied *ex situ* on cycled $LiFePO_4$ electrodes where mapping of the different components were obtained and immobilisation of lithium as micrometric clusters was evidenced and correlated to the aging of the electrode[41].
The morphological and structural changes in the materials of interest will be investigated ***in operando*** using the **SAMBA and ROCK beamlines of the synchrotron SOLEIL**. For example, in the case of carbon nanotube carpets, the initial formation of metallic oxides on the CNT surface will be first investigated *ex-situ* using X-ray absorption and fluorescence spectroscopies to make further correlation with the *in operando* analysis. A specific constant flow electrochemical cell has been tailored in LAMBE to investigate the electrolyte-electrode interface using X-ray analysis upon electrochemical solicitation. In operando infrared spectroscopy is also available at X/PMC and leads to chemical information on both the bulk lithiation process of the electrode and the chemical evolution of the electrode/electrolytes interface.[42]

2.3. WP2 - Resource Center

One key action of MOMENTOM is the creation of a Resource Center to facilitate exchanges between academic and industrial partners, to support the design and fabrication of unique devices for scientific,

[41] Habrioux, A. *et al.* Nuclear microanalysis of lithium dispersion in $LiFePO_4$ based cathode materials for Li-ion batteries. *Nucl. Instrum. Methods Phys. Res. Sect. B Beam Interact. Mater. At.* **290,** 13–18 (2012)
[42] D. Alves Dalla Corte, G. Caillon, C. Jordy, J.-N. Chazalviel, M. Rosso and F. Ozanam, Adv. Energy Mater. 6, 2016, 1501768

training or outreach purpose, and to favour the sharing of equipment. ***In fine*, its objective is to ensure the future of the MOMENTOM project by developing sustainable relations with industrial partners.**
This Resource Center will be managed by P. Gaucher, an expert of materials science who has experience in the coordination of European projects and in the development of projects with industrial partners (CV in **annex 3**). P. Gaucher will lead the aspects related with valorisation, promotion of the laboratories at the European level. Relations with industrial partners will rely on F. Plais (CV in **annex 3**), currently in charge of the industrial valorisation service at Ecole Polytechnique. A. Aukauloo and H. Remita will lead the educational and dissemination aspects. The Center will also include a recruited engineer for the daily technical operations at the prototype platform.

2.3.1. Prototyping platform (WP2.1.)

Within the Resource Center, the objective of the prototyping platform is dual:
i) To develop specific scientific tools to characterise materials *in operando*. The intent is to favour the development of devices allowing to assess the behaviour of advanced material in working conditions by coupling to characterization facilities like Soleil synchrotron. Here are few examples of such devices:
- *In operando* Raman micro-spectroscopy of the membrane electrode assembly (MEA) of a fully operating PEMFC. Automated system will allow a depth profiling of the fuel cell by an appropriate positioning of the micro-spectroscopy laser focal point for MEA catalytic layer spectroscopy.
- *In operando* X-ray diffraction for Li-ion batteries, to detect cathode material evolution and potential failure upon cycling or overcharge …

ii) To help laboratories building lab-scale demonstrators for potential industrial partners and for divulgation purpose: The prototyping platform will have expertise and human resources to help building lab-scale demonstrators incorporating the advances made during the research program. While materials will be developed at the laboratory scale (button cell,…), the demonstrators will include the electronics, the interface with external sources of energy, the measuring of power efficiency *i.e.* all the required elements to present a fully working device and easily evaluate its efficiency. Examples of such demonstrators might include:
- A hydrogen storage device coupled to a photocatalytic process;
- A packaged power source with embedded electronics (current regulation and energy measurement);
- Small photocatalytic reactors based on modified semiconductors for H_2 production by solar light;
- Small "Hydrogen full value chain" demonstrators for educational purpose.

The prototyping platform will be housed by the "Fabrique" at CentraleSupelec taking benefit from its facilities: *3D-prototyping (Fab Lab), Electronic laboratory with CAO tool, printed circuit technology and measurements facilities, Laser-cutting tools, packaging and assembly techniques*…. In terms of human resources, beside the three permanent people already present at the "Fabrique", a full-time engineer will be recruited, funded by MOMENTOM, to deal with the laboratory projects to be developed at the platform.

2.3.2. Valorisation and industrial relations (WP2.2.)

The Resource Center will develop the scientific and technological skills obtained by MOMENTOM's teams, at the academic and industrial levels. For academic aspects, the objective is to go beyond the classical publishing or participation to conference by proposing a joint expertise to potential academic partners, e.g., at the European level. MOMENTOM ideas/technologies will be presented in dedicated events to meet potential cooperation partners (for instance the Brokerage events organised by the European Commission in the field of Energy), to contact a wide spectrum of companies, universities and researchers from Europe and to foster the creation of **consortia** for the upcoming **Horizon 2020 Energy calls**.
For industrial aspects, the Resource Center will be an interface between the industrial partners and the MOMENTOM involved laboratories. In this case, the experience from F. Plais will be of strong help to develop **relations with industrial partners**. To promote the results of MOMENTOM teams toward industrial partners and settle new partnerships, different strategies are foreseen:
- **Organisation of "Petits-déjeuners university-industry":** specific industrial partners will be invited and recent results and demonstrators from academic partners and specific needs from industry will be presented. They could be organised jointly with the Energy programme of the University Paris-Saclay.
- **Prospection of PMEs in the field of energy**: information about MOMENTOM and results will be sent to partners (including but not limitative, SATT as they receive solicitations from industrial partners, Optics Valley as their role is to strengthen the network of SMEs in the Saclay area…).

- **Review of background Intellectual Property assets** hold by institutions and related to MOMENTOM. Based on these assets (patents, softwares or know-how), technological offers will be published on MOMENTOM and "PWI FCS-SATT" websites and presented in various go-between events.
- **Visits of laboratories:** several MOMENTOM teams manage top level characterisation tools and platforms whose visit could be proposed to the industrial partners registered to our "Club of Partners" – even if "free of charge", this formal registration will help to create and render visible a large community–. Dedicated "Doctorant-conseil" missions could be set-up for the organization of these "lab-discovery events".

MOMENTOM will rely on the experience of the teams which have already led to the emergence and success of start-ups: NanoE and NextMat born at CentraleSupelec, TeraTonics associated to LCP, UPSud... The Resource Center will not substitute existing schemes such as the different incubators (Incuballiance, CentraleSupelec incubator, CEATech) for housing start-ups at their very first stage of development. It will act as an interface between students, laboratories and these entities to favour the emergence of innovative concepts. For instance, innovation projects could be proposed to students or an expertise network could be settled with the objective to help students to build their own company project.

2.3.3. Education program (WP2.3.)

This action is crucial in pertaining a long-term project on the energy issues in the realm of Paris-Saclay. Paris-Saclay has a wide offer as compared to other energy centres in France or abroad. At the **Bachelor (Licence)** level, 3 training programs are dealing with renewable energies. At the **Master** level, specific training programs on renewable energy are proposed by UPSay.[43] Many members of the consortium are involved in teaching in these Bachelors and Masters. MOMENTOM will propose complementary activities to gather the academic and industrial worlds on defined targets:

- **Trans Disciplinary Scientific Meeting** will gather colleagues embarked on this project with different specialities (energy solar conversion, batteries, hybrid materials, electronics, theory and modelling, economic and social issues for the environment) to present and explain the basics of their research field and the actual breakthroughs that are expected. We strongly believe that knowing each other will help to build a more committed community around this paramount task.
- **Specialised courses** will be proposed to technicians and engineers of industrial partners and students in professional programs. The scientific, technical and economic issues will be addressed to build a long-standing partnership between the academic and the industrials. At the technician level, classical courses will focus on technological aspects (fabrication, operation, maintaining…). At the engineer/master level, the courses will integrate all the relevant aspects of a technology from the industry point of view including economic aspects, with a multidisciplinary approach around a device. For instance, we will propose a course on the "Fuel cell device" (36 hours = 1 week), from basic principles to components, fabrication, operation and economic aspects of fuel-cell general use, with laboratory practice. Such a course could be transposed to other technologies**.** These one-week specialised courses are to be funded by industrial partners. Previous experience indicates that a 15-20 k€ funding can be expected from an industrial partner to train 12 students during a week. This will participate to the long-term outcome of MOMENTOM.
- **An Annual International Summer School "New materials for the Energy of Tomorrow"** will answer the growing need of graduate students and researchers to be acquainted to a targeted field and its instrumental techniques. Besides classical programs in chemistry, physics or biology, it will teach specialised research practices and techniques from our consortium expertise. This will contribute to spread good research practices. Such an event could also help to tie new collaborations with international groups.
- **MOOCs** (massive open online courses): Tailored courses on materials for energy focused on materials for hydrogen (formation, use and storage), solar energy conversion, and materials for energy storage. They will also include theoretical approaches and modelling to provide methodology background to experimentalists.
- **International MOMENTOM Congress (IMC) every two years** whereby colleagues from all round the world will be invited to share their findings and results.

2.3.4. Dissemination (WP2.4.)

Beside standard dissemination – participation to international congresses, scientific publications…–, MOMENTOM will drive specific actions (see above for the valorisation at the European level) with the objective to communicate on the scientific advances and breakthroughs obtained during the project:

[43] The list of the Master courses dealing with renewable energy at UPSay is given in **annex 5**.

i) Annual MOMENTOM Workshop will bring academia and industry together to discuss basic research and technological issues and social sciences (including economics) aspects. These meetings will be a privileged place to encourage both academics and industrials to establish long-term projects such as ANR proposals. They will be complementary to those organised by the initiative on Energy of UPSay.
ii) Science-to-Society actions: An important part will be dedicated to present these new technologies and their potential impact on society towards the general public:
- Participation to the "Fête de la Science" by "open doors" for two to three days per year, allowing classes and public visit the Competence Center and research laboratories with demonstrations on new energies.
- Demonstrations as a part of the program "un chercheur - une manip" at the Palais de la Découverte (A museum of Science in Paris) on solar hydrogen production and its use for small vehicles.
- At Maison d'Initiation et Sensibilisation aux Sciences (MISS),[44] organisation of a workshop on renewable energy: a small photocatalytic reactor based on modified semiconductors will be built for hydrogen production by solar light (H_2 production followed by mass spectrometry and gas chromatography) and small hydrogen vehicles based on H_2 fuel cells.

2.4. Involved resources and justification of the requested budget

2.4.1. Budget

		Nature	Phase 1	Phase 2	TOTAL
WP1 Challenges	Post-docs (11 man.months)	Salary	220 000	385 000	605 000
	Master students (16 * 6 months)	Grant	26 500	26 500	53 000
	Research support (5000 € /post-doc/year)	Operational budget	20 000	35 000	55 000
WP2 Resource center	Prototyping platform engineer (2 years)	Salary	40 000	60 000	100 000
	Prototyping platform functioning budget	Operational budget	80 000	80 000	160 000
	Industrial relations responsible secondment (20% - 2 years)	Sub-contracting	20 000	30 000	50 000
	Industrial relations functioning budget (workshops, meetings, travels)	Operational budget	23 500	23 500	35 000
	Education functioning budget (courses organisation, summer school, …)	Operational budget	15 000	15 000	30 000
TOTAL			**445 000**	**655 000**	**1 100 000**

Co-funding:
In view of MOMENTOM task force (688 men.months; see annex 4) the implication of parent organization in MOMENTOM is considerable. Moreover, most of MOMENTOM teams run funded projects (ANR, H2020 projects, industrial collaborations…)[45] related to MOMENTOM, not listed here since they have been obtained without explicit link to MOMENTOM. Co-funding from industrial partners will be a major outcome of MOMENTOM.

2.5.2. Justification of the requested budget

WP1 budget. 713 000 €

- **Post-docs (11 men.months). 605 000 €.** Post-docs will implement the research actions selected in MOMENTOM challenges and will act as links between involved laboratories. **During Phase 1**, there will be only **4 post-docs** recruited on specific already defined topics. During **Phase 2**, **7 post-docs** will be recruited to increase significantly the workforce.
- **Research support (5000 € /post-doc/year). 55 000 €.** A budget will accompany post-doc recruitments for consumable expenses, specific characterization costs, personal computers and travels of post-docs to participate to international congresses. This last point is crucial for MOMENTOM impact.

[44] http://www.ladiagonale-paris-saclay.fr/nos-actions/miss/
[45] ANR DYNAWIN ('spectroscopy at interfaces'), SLIMCAT ('material design'), etc…-, European projects (FET Open, RIZE…), collaborations with industrial partners (Air Liquide, ArevaH2Gen, EDF, IFPEN, Renault…).

- **Master students (16 * 6 months). 53 000 €.** Master students represent a possibility to pre-recruit candidates for PhD and a means of supporting exploratory projects for which funding is difficult to find.

WP2 budget. 340 000 €

- **Prototyping platform engineer (2 ½ years). 100 000 €.** After the settling of the "fabrique" entity at CentraleSupelec by half of 2017, an engineer will be recruited on a full time position till the end of the project. The person recruited will be in charge of developing new prototypes and demonstrators with the laboratories using the different facilities of the "Fabrique" entity.
- **Prototyping platform functioning budget. 160 000 €.** Budget will be dedicated to build prototypes for research, for demonstrators and for educational experiences. They will be made from 3D-prototyping or machining, and include electrical connection and circuits and specific packaging in case of educational kits. The mean cost for operational small prototypes and demonstrators is estimated between 3 and 10 kEuros.
- **Industrial relations responsible secondment (2 ½ years). 50 000 €.** F. Plais (see CV in annex 3), apart of his present position as the head of the valorisation service at Ecole Polytechnique, will spend 20% on his time during the last two years and a half on prospecting potential industrial partners for MOMENTOM consortium. Sub-contracting this action will cover his salary for the period of time dedicated to the project.
- **Industrial relations functioning budget. 47 000 €.** The participation to H2020 events will represent typically 1500-2000 €/year representing two travels/year for the Resource Center director. Industry-university meetings will also be organised with invited industrial partners (petits-déjeuners or annual workshops) and small and intermediate companies in the field of energy will be prospected.
- **Education functioning budget. 30 000 €.** A MOOC and the Annual Summer School on "New materials for the energy of Tomorrow" will be proposed at an attractive price to a vast community of PhD/master students from France and abroad, a crucial for the international visibility of the University Paris-Saclay.

3. Expected impact of the project

3.1. Impact on Université-Paris-Saclay visibility and research

This trans-disciplinary project gathering well recognised teams with complementary expertise will strengthen the skills and will increase the leadership and visibility of UPSay in this highly competitive field in France and at the international level. For instance, our consortium will allow UPSay to gain visibility in national networks such as RS2E in which it is currently poorly represented. The Resource Center will be instrumental for technological transfer and for development of collaborations with industrial partners.
MOMENTOM will also impulse new ambitious national (such as ANR, ADEME) and European projects (such as FET Open, European network type COST -European Cooperation in the field of Scientific and Technical Research-, RIZE and ITN -Innovative Training Networks-). Such a concentration of academic and industrial laboratories working in the field of energy on the plateau of Saclay is quite unique and will impulse to this project an international dimension. The training actions will participate in the attractivity of UPSay and its national and international visibility. Finally, the outreach actions of MOMENTOM will contribute to the public education and the acceptation and integration of new energies in every-day life.

3.2. Structuring role of the project

MOMENTOM is in the heart of two transversal initiatives of Paris-Saclay "Energy" and "Materials". This trans-disciplinary project will gather teams with complementary expertise in Material Science, Chemistry, Physics, and Economics from different departments of UPSay (Chemistry, PhOM and SHS). These teams will interact through workpackages, training and dissemination actions and/or workshops. Indeed, the Trans Disciplinary Situation Room as well as the MOMENTOM workshop and congress (IMC) will be very important in structuring the community around materials for energy considering social and economic aspects related to "new energies". MOMENTOM will interact with the project GRID4EARTH (as part of the program MISTIGRID) in the frame of the transversal initiative on Energy. Finally, MOMENTOM will help to build a network of academic laboratories with different industrial groups and Start-ups present at the Plateau de Saclay. Also it is worth noting the important role of the MOMENTOM Resource Center: This tool will act as a visible desk centred on energy topics between UPSay laboratories and industrial partners.

3.3. Societal impact, economic and capacity to respond to the stakes of the challenge

We expect that our research activities will lead to original and breaking solutions for energy conversion, use and storage considering economic issues. The Resource Center will be the interface of our community with the economic and social players. The different actions proposed in WP2 will favour strong interactions with industrial partners on both research and education, and facilitate the emergence of collaborative projects and will favor start-up creation. The Resource Center will thus help accelerating the valorisation of scientific results and might thus become a powerful innovation factor. Finally, the different outreach activities will contribute to knowledge of new energies for the new generation and large public in general as well as their acceptability and integration in their every-day life.

Impact on involved partners:
MOMENTOM will reinforce and extend the experience of each partner in his field of excellence and, due to the multi-disciplinary character of the project, will give them access to novel skills and to new facilities. The possibility for PhD students and post-docs to train easily in other laboratories without escaping from their original field also constitutes a strong added value. MOMENTOM will not only enable to exchange good practices and improve current ones, but will also help generating new ideas and promoting innovation among partners. It will thus contribute to gain an European leadership in a key scientific area, materials for green energy applications and economic impacts of these technologies.

Impact on the scientific community
Top level results in short time are expected in the challenges identified at the core of partners' expertise and excellence. The shared skills and facilities will allow for shortening the time needed for experimental development and characterisation, and increasing the level of research. In particular, the access to specific tools (like the Nuclear probe or TeraHertz spectroscopy) will facilitate the emergence of new results. The additional resources provided by MOMENTOM will accelerate the development of more mature research topics and will allow dedicating resources on more exploratory projects. The prototyping platform will help laboratories to build specific research tools and small demonstrators as a showcase of scientific breakthroughs. Such developments will beneficiate to the whole MOMENTOM community and might also favour the creation of innovative research tools. Moreover, the organisation of special events will gather different kinds of public: renowned scientists but also non initiated public as students coming from all countries across Europe. In particular, an **open workshop "New Materials for the Energy of Tomorrow"** will increase young people awareness on scientific aspects in the concerned domains and the need to make European cooperation.

4. Midterm (1.5/3-year) perspectives of the project

4.1. Scientific perspectives

The building of the project (with numerous preparation meetings) has favoured the reciprocal knowledge of involved partners and has already generated a dynamics toward a fruitful cooperation. We expect already several ANR national projects to be mounted for the 2017 generic call (in fall 2016) and all along the MOMENTOM project. We also expect that the strengthening of our expertise, the excellence of results obtained within MOMENTOM and the various actions of the Resource Center will promote the participation of MOMENTOM teams to H2020 projects. In this sense, the MOMENTOM support to specific research actions reflects our strategy to choose topics already at the cutting edge in the international competition.

4.2. Financial perspectives

MOMENTOM aims at favouring the future implication of industrial partners. A timescale of 3-years is reasonable to settle sustained relations between academic laboratories and identified partners, thanks to the creation of the Resource Center. Several parallel funding schemes will be explored to maintain the dynamics of research and collaboration triggered by MOMENTOM: CIFRE PhD theses, industrial Chair (through ANR scheme or corporate sponsorship), direct contracting, ANR and European projects for which, again, the Resource Center will be decisive for promoting MOMENTOM teams during Brokerage events. We also consider that our education program toward companies, in particular the specialised courses, will generate incomes that will facilitate the sustainability of the Resource Center. Finally, considering the forces present in MOMENTOM and at the regional level, we will propose a new "Domaine d'Intérêt Majeur" (DIM) (funded by the Ile-de-France region) on hydrogen technologies and green energies for transports.