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PROJECT FINAL REPORT

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Project acronym: MOLSURMOF

Project title: MOlecular Loading and SURface anchoring of Metal-Organic Frameworks: a training and career development action

Funding Scheme: Marie Curie Actions - Intra-European Fellowships (IEF)

Starting date: 16th March 2012; **Duration**: 24 Months

Period covered: **from** Month 1 **to** Month 24

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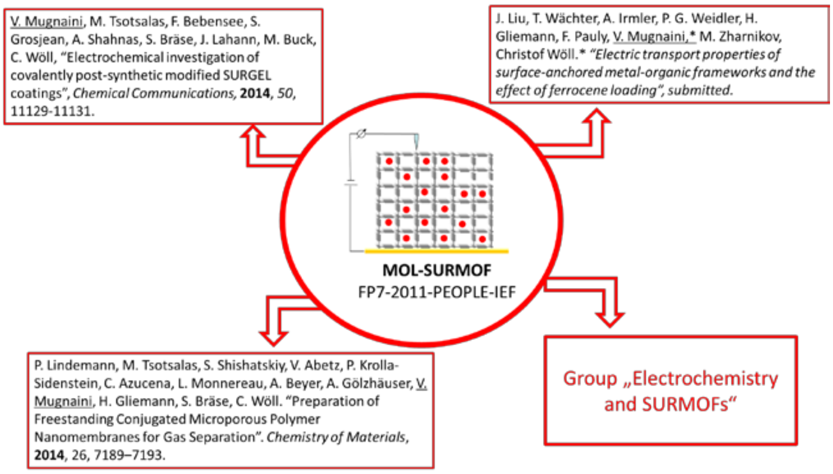
Final publishable summary report

1. Executive summary of the project

The main **goal** of the **MOL-SURMOF** project granted in the frame of the Marie Curie IEF Action, was the investigation of the electronic properties of metal-organic frameworks anchored to solid surfaces (**SURMOFs**) before and after their **loading** with organic **electro-active molecules** (MOL) to **shed light on the charge transport mechanism** of these materials, such surface anchored hybrid metal/organic structures that bear a huge potential in electronic devices.

Metal-organic frameworks (MOFs), crystalline and porous materials based on the coordination of metal ions and organic linkers, have been extensively studied but mainly for gas storage, separation and catalysis applications. In the last couple of years, however, they have been attracting much attention as potential candidates for novel electronic devices, thanks to their tailorable chemistry, crystallinity and porosity. Nevertheless, a thorough experimental characterization of the electrical transport properties and charge transport mechanism of these materials has so far been rather problematic due to the challenges in their processing as robust, crystalline and oriented thin films. In fact, from the point of view of setting up an experiment to measure electrochemical properties, either conductivity or impedance, for example, **powder MOFs** might **present a challenge**. Indeed, these types of experiments need the robust anchoring of the species under study, to an electrode. The **electrode fabrication** can therefore be considered as the **main limitation** for the widespread use of this application. **Within this context**, the approach proposed in the frame of this proposal, *i.e* the use of surface anchored metal-organic frameworks (SURMOFs) and molecularly loaded SURMOFs (MOL-SURMOFs) grown on template surfaces by means of the stepwise liquid phase epitaxy (LPE) method, represents a huge step forward in this field and contributed to reinforce a **completely new field of applications** for these materials. Indeed, SURMOFs and MOL-SURMOFs can **themselves** be used as **robust solid electrodes** and hence integrated in electrochemical cells or Hg-based tunneling junctions. By following these two experimental approaches, it has indeed been possible to measure the electrical properties and to elucidate the charge transport mechanism of these novel materials.



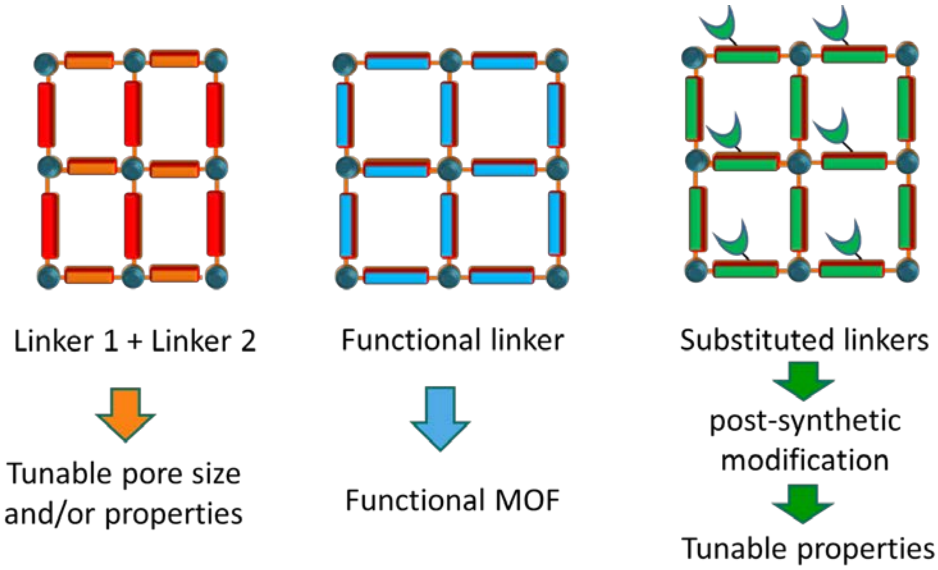
We believe that the knowledge of the factors influencing the charge transport mechanism in SURMOF films, both as pristine and after incorporation of a guest molecule, paves the way towards the exploitation of their predicted and foreseen large potential for applications in electronic devices. To the best of our knowledge this is the first study of this kind and as such it will with no doubts substantially promote the understanding of electric transport properties of MOFs (one manuscript submitted and one in preparation).

Additionally, in the frame of this project, cyclic voltammetry was shown to be the method of choice for the investigation of the film quality of SURMOFs and MOL-SURMOFs but also of surface anchored purely organic gels (**SURGELS**) and purely organic membranes (two published manuscripts).

2. A summary description of project context and objectives

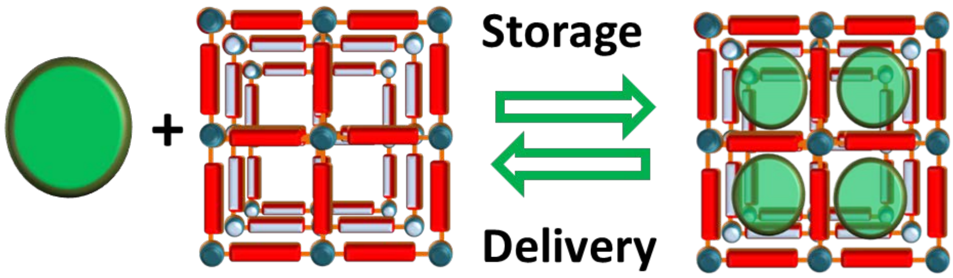
State of the art. Metal-organic frameworks (MOFs) are crystalline and porous materials based on the coordination of metal ions and organic linkers.[1] Their porosity depends on the distance between the metal ions, hence on the length of the organic linker. Indeed, it has been shown in a pioneering work of the group of O. Yaghi *et al.*[2] that by changing the length of the organic linker isoreticular structures with pore sizes ranging from less than 1 nm to 12 nm can be prepared. Undoubtedly, their porosity and hence their capability to host and release nano-objects (*i.e* gases, nanoparticles, small molecules as well as proteins) has been their most exploited property, towards the preparation of sensing devices, drug carriers/deliverers, fuel cell components, to name a few.[3]

Moreover, skilled chemists have shown that the range of possible linkers and metal ions, as well as the combination of the two, is almost endless, as demonstrated by the fact that thousands of MOF structures have been reported up to date.[4] The possibility to use almost any organic linker or inorganic node allows for the tuning of the function of these polymeric materials, *i.e*. the MOFs' tectons may act not only as structural moieties but may also embed a specific property. Recently, organic tectons bearing electroactivity have been extensively tested, in order to achieve specific electronic properties for the resulting MOFs.[5]



Scheme 1. Examples of the possible organic tectons for the preparation of MOFs.

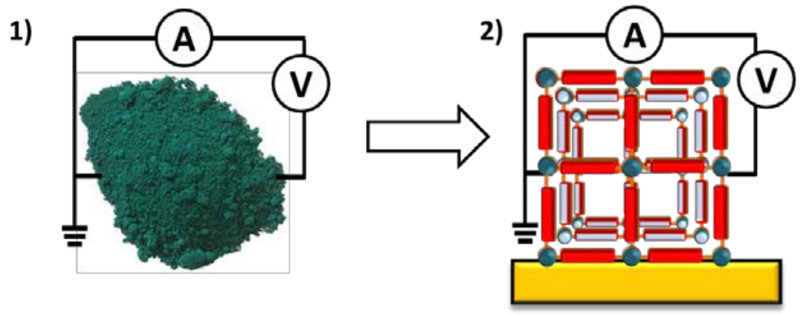
However, the synthetic modification of the organic linker is not the only path to achieve tunable electronic properties: as shown in the work carried out in the frame of this Marie Curie funded project, interesting electric properties can also be achieved by insertion of electroactive guest molecules in the framework's pores.[6]



Scheme 2. The green sphere represents a guest molecule that is reversibly hosted in the pores/void spaces of a metal-organic framework.

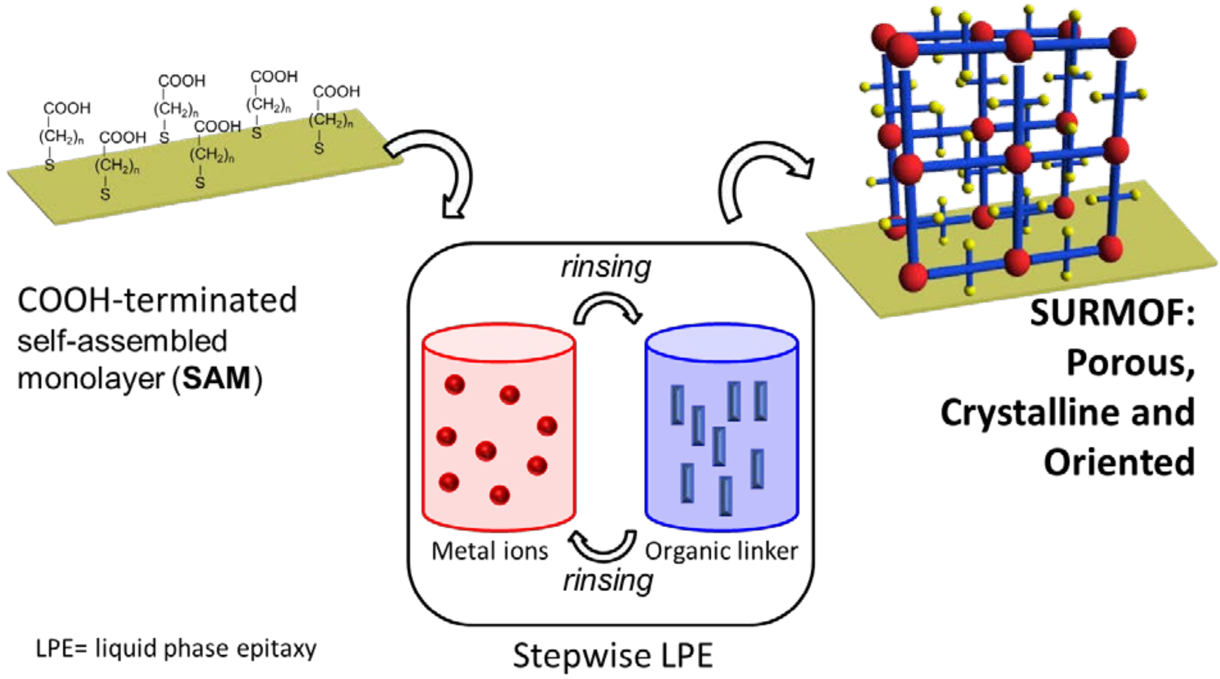
Generally speaking, the possibility to either use **(multi)functional building blocks** or change the pore size and **add a non-native function by pore modification** make these materials **highly versatile and relevant** in several applications, including electronics.

For the realization of actual electronic MOF-based devices the deposition on a supportive surface as homogeneous, defect free and robust coating appears as the fundamental pre-requisite (Scheme 3), and most of the time, a great challenge.[7]



Scheme 3. 1) Electric connections in a powder/particulate system. The major drawback is the experimental handling. 2) Same electric connections in the case of a surface anchored MOF: being supported on a surface the assembly is straightforward. The SURMOF itself can be used as electrode.

MOFs - and related materials - offer in this frame great prospects since it has been demonstrated that many of them can be deposited as oriented and crystalline porous on surfaces/solid supports, this being the first step towards the implementation in devices.[8] Therefore, towards the actual use of MOFs in electronics and specifically for their future implementation in devices, they have to be robustly anchored on solid supports, *i.e*. on surfaces, and they have to maintain their unique properties: crystallinity and porosity: This can be achieved following the methodology introduced by Fischer, Wöll and co-workers and based on room temperature liquid phase epitaxy (Scheme 4) and followed in the frame of this project.[9]



Scheme 4. From left to right: conductive template surface passivated with a self-assembled monolayer (SAM) of –COOH terminated thiols. In the middle: the surface is immersed in the solution of metal ions (in red), rinsed to remove the excess of not specifically bound metal ions and then immersed in the solution of the organic linker (in blue). The excess of unbound organic linkers is removed by rinsing. This step (named cycles) is then repeated as many times as desired. The number of repeated times is responsible for the surface anchored MOF thickness.

2D and 3D surface anchored metal-organic frameworks (SURMOF) have therefore been prepared according to the established liquid phase epitaxy (LPE) procedure and then their void spaces loaded with small electroactive guests, giving MOL-SURMOF films.

Objectives. The electrochemical, electric and charge transport properties of SURMOFs and the molecule-loaded MOL-SURMOFs have been thoroughly studied with accomplishment of the following objectives:

1) Preparation of surface anchored metal-organic frameworks (SURMOFs) by means of the stepwise liquid phase epitaxy methodology on polycrystalline gold functionalized with an organic self-assembled monolayer;
2) Loading of the pores with functional small molecules, such as ferrocene;
3) Investigation of the obtained molecular loaded SURMOFs (MOL-SURMOFs) by routine characterization methods, mainly cyclic voltammetry
4) Investigation of the charge transport and electric properties of SURMOFs and MOL-SURMOFs;
5) Electrochemical characterization of purely organic porous coatings (POFs and SURGELs).

By investigating the electronic properties of **surface anchored MOFs and related frameworks**, *i.e.* generally speaking of 2D and 3D polymeric porous coatings, before and after the decoration of their pores with molecules bearing a specific non-native electrochemical response, the MOLSURMOF project has actively contributed to shed light on the electric properties of a representative SURMOF series responding to the challenging demand of the scientific and industrial community of **novel molecular based electronics devices.**

The work carried out by the fellow in the frame of this project led to the following publications and submitted manuscripts:

J. Liu, T. Wächter, A. Irmler, P. G. Weidler, H. Gliemann, F. Pauly, V. Mugnaini,* M. Zharnikov, Christof Wöll.* *"Electric transport properties of surface-anchored metal-organic frameworks and the effect of ferrocene loading", submitted.*

P. Lindemann, M. Tsotsalas, S. Shishatskiy, V. Abetz, P. Krolla-Sidenstein, C. Azucena, L. Monnereau, A. Beyer, A. Gölzhäuser, V. Mugnaini, H. Gliemann, S. Bräse, C. Wöll. "Preparation of Freestanding Conjugated Microporous Polymer Nanomembranes for Gas Separation". *Chemistry of Materials*, **2014**, 26, 7189–7193.

V. Mugnaini, M. Tsotsalas, F. Bebensee, S. Grosjean, A. Shahnas, S. Bräse, J. Lahann, M. Buck, C. Wöll, "Electrochemical investigation of covalently post-synthetic modified SURGEL coatings", *Chemical Communications,* **2014**, *50*, 11129-11131.

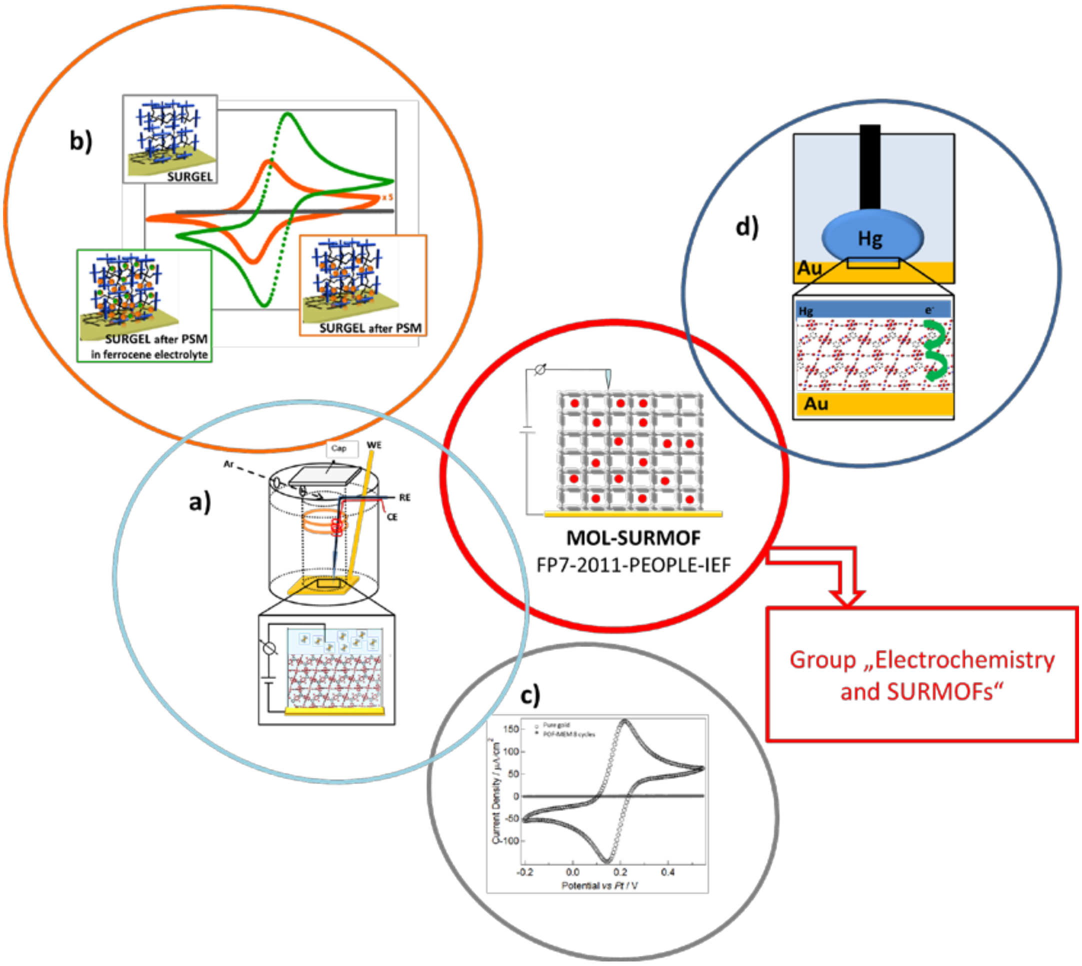
Two more manuscripts are in preparation.

Additionally, the dedicated work of the **fellow** in the field of electrochemistry made her being chosen as **leader** of the **group** dedicated to "**Electrochemistry and SURMOF**" at her host research institute.

3. Description of main achieved results

The main achievements of the MOL-SURMOF project, as schematized in Scheme 5, are the following:

1. the establishment of a protocol to investigate porous coating by means of cyclic voltammetry using the home-made set-up introduced and optimized by the fellow herself (a);
2. the investigation of the electrochemical properties of SURGELs as prepared and after the introduction by post synthetic modification (PSM) of en electroactive ferrocenyl moiety (b).
3. the investigation of the film quality of purely organic membranes by means of cyclic voltammetry (c);
4. the ***integration of a representative crystalline and porous metal-organic framework*** - obtained as surface anchored oriented and crystalline films (SURMOFs) of variable thicknesses by means of the stepwise liquid phase epitaxy - in ***mercury tunneling junctions*** and the ***measurements of their electric transport properties*** (d).



Scheme 5. Schematic representation of the main achievements reached through the implementation of the MOL-SURMOF project and the accomplishment of the proposed objectives. a) Protocol for the use of a home-made electrochemical cell for the investigation of SURMOF and MOL-SURMOF films. b) Investigation of the electrochemical properties of surface anchored organic films (SURGELs), before and after their post-synthetic modification (PSM) by thiol-yne click chemistry.[10] c) Investigation of purely organic films (POFs).[11] d) Integration of SURMOF and MOL-SURMOF films in a Hg-based tunnelling junction.[12] Additionally the group named "Electrochemistry and SURMOFs", led by the fellow, has been established in the host institution.

1. Establishment of a protocol to investigate porous coating by means of cyclic voltammetry using the home-made set-up introduced and optimized by the fellow herself.

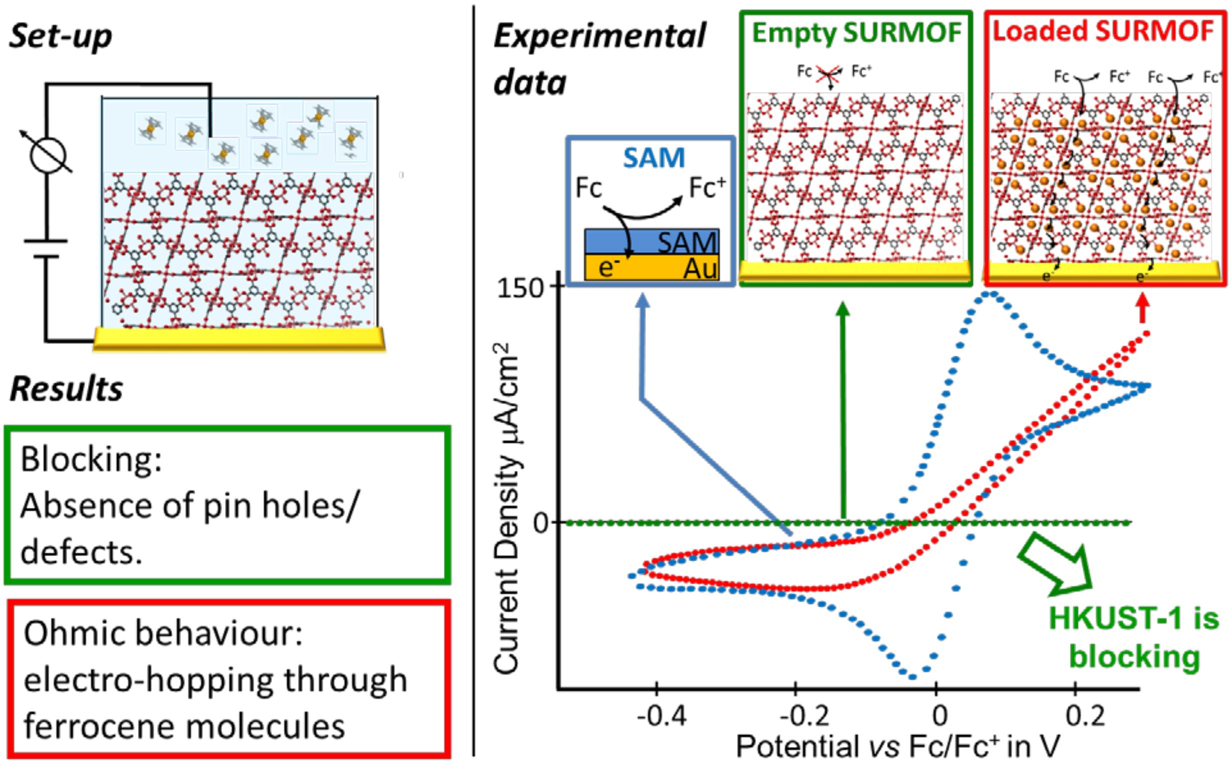
The fellow focussed her work on the *1)* use of a **standard three electrodes set-up**; and *2)* optimization of a **home-built electrochemical cell** specially designed for the study of SURMOFs and MOL-SURMOFs. In this set-up, SURMOFs and MOL-SURMOFs can themselves be used as working electrodes. The main drawback resides in the low stability of these films under the generally used electrochemical working conditions. Since standard electrolytes and solvents generally used in electrochemical experiments led to a partial disruption of the sample crystallinity, the fellow moved to the use of a room temperature ionic liquid, the 1-butyl-3-methylimidazolinium bis(trifluoronethylsulfonyl)-imide ([BMIM] [NTf_2]), and proved the stability of the used SURMOF in such a solution by means of both X-ray diffraction (XRD) and infrared reflection absorption spectroscopy (IRRAS), hence establishing the use of this ionic liquid as standard for the study of SURMOFs. Other ionic liquids were also tested, but in none of them the used SURMOF showed to be stable enough to allow for the desired investigations to be carried out. She used this set-up for the accomplishment of objectives 2 and 3 (see below).

In addition, she studied the SURMOF formed by the coordination of trimesic acid and copper acetate (HKUST-1) as pristine film and after the incorporation of ferrocene on the 9-carboxy-10-(mercaptomethyl)triptycine SAM. This study can be considered as a preliminary investigation that then led to the accomplishment of objective 4.

The awardee investigated the film quality as well as the role of the ferrocene molecules incorporated inside the framework's pores on the electrical conductivity.[6a] To gain insight into the film quality, she dissolved ferrocene as electroactive probe inside the ionic liquid solution and carried out cyclic voltammetry experiments on the SAM, the HKUST-1 SURMOF and the MOL-SURMOF formed by ferrocene in HKUST-1. The results are schematically shown in Figure 1.

In the case of the SAM the redox of the ferrocene dissolved in the ionic liquid is recorded. In the case of the SURMOF, instead, no redox is observed: indicating that the SURMOF film acts as a blocking barrier impeding the ferrocene dissolved in the ionic liquid to reach the bottom part of the film, i.e. the conductive gold electrode. The ohmic-like behaviour after ferrocene loading is instead an indication of a charge hopping mechanism mediated by the ferrocene molecules immobilised inside the pores.

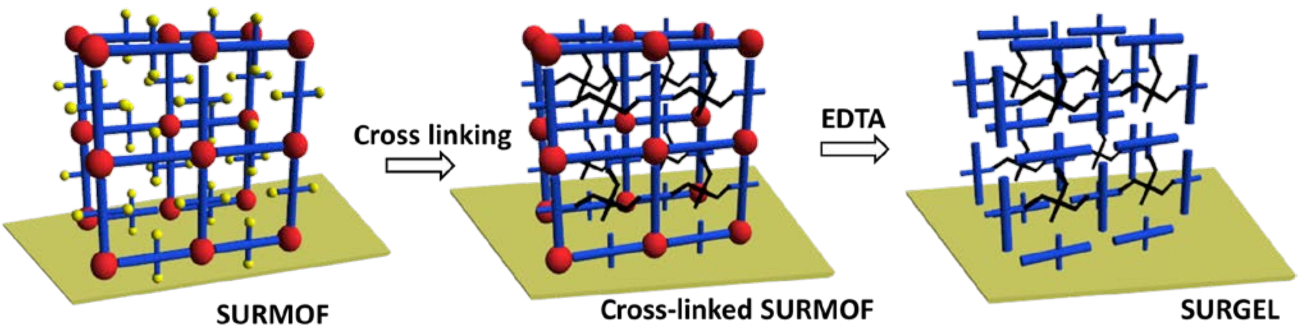
Figure 1. Set up, experimental data and results as described in the main text.



A similar study was submitted for publication during the submission of this proposal.[6a] Therefore, in order to make the work of the fellow innovative and hence suited for publication, she studied the diffusion of the ionic liquid used as supporting electrolyte by means of quartz crystal microbalance. This investigation is the first of this kind, and it is believed that it will have a great impact in the scientific community, since it has so far only been hypothesized that the ionic liquid can diffuse inside the MOF structures. The manuscript will be ready for submission at the time of submission of this report.

2. Investigation of the electrochemical properties of SURGELs as prepared and after the introduction by post synthetic modification (PSM) of en electroactive ferrocenyl moiety.

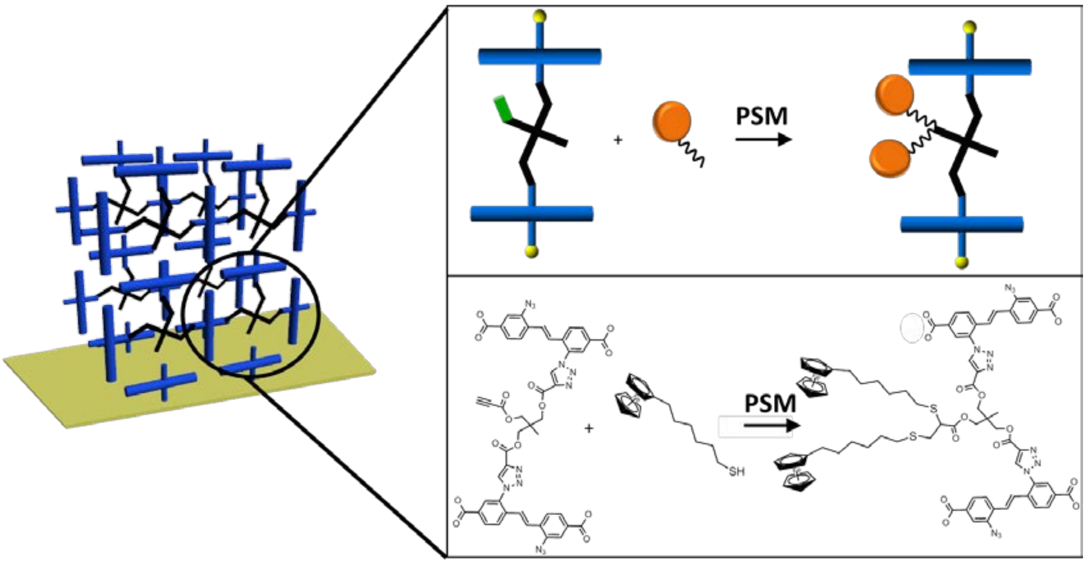
SURGELs[13] are purely organic, porous, and covalently bound gels obtained from SURMOFs that bear a large potential in biological applications thanks to their 1) enhanced water stability and 2) lower toxicity thanks to the absence of metal ions in their structure (Scheme 6). They were first prepared at the end of 2012 by a colleague of the fellow working in the same laboratory. For this reason, the investigation of their electrochemical properties could not have been foreseen during the writing of the Marie Curie proposal.



Scheme 6. From SURMOF to SURGELs. Adapted from reference 13.

The fellow undertook the electrochemical investigation of this **SURGEL** porous coating and found that it is a **homogeneous defect and pin-holes free coating**.

Additionally, taking advantage of her background in chemistry, she was able to modify the structure of the SURGEL *via* covalent post-synthetic modification (PSM),[10] with a reaction based on thiol-yne click chemistry employing the alkyne moieties still available after the SURGEL formation (Scheme 7).

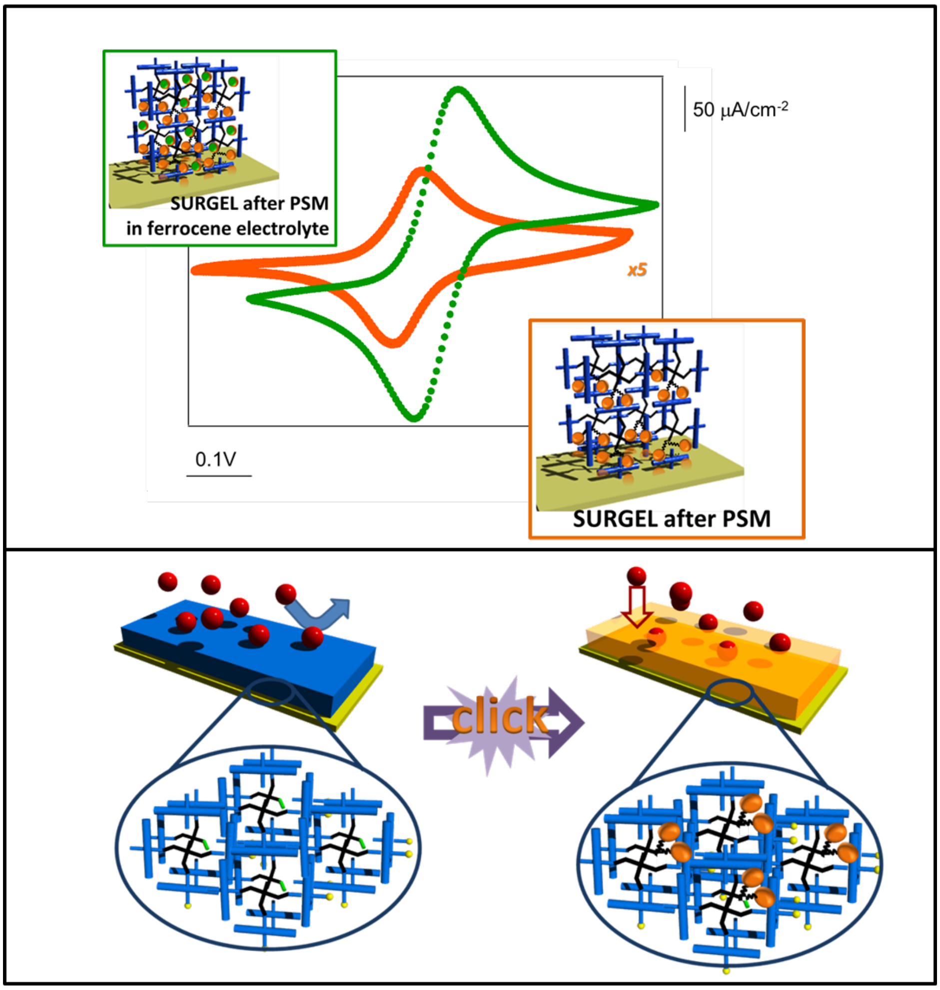


Scheme 7. On the left, the SURGEL structure. On the right: zoom in the residues involved in the PSM. Adapted from reference 10.

The success of the PSM process, as confirmed by a thorough spectroscopic characterization (IRRAS, XPS), demonstrates that SURGELs provide a robust platform for the attachment of functional moieties and hence the fine tailoring of the properties of these 3D open polymeric coatings.

By the introduction of a ferrocenyl derivative she could investigate the electrochemical properties of the modified SURGEL. By means of cyclic voltammetry, it is demonstrated that the ferrocene, covalently bound to the SURGEL via a flexible alkyl linker, can be reversibly oxidised and reduced. The reduction and oxidation peaks appearing at different potentials suggest that these moieties have some degree of mobility, as indeed expected from their rather flexible anchoring chain to the SURGEL framework.

Additionally an increased permeability of the porous coating after PSM (Scheme 8) was found: an unexpected result that deserved publication in a high impact factor journal.[10] Indeed, in the case of PS modified SURGEL, much higher currents and larger separations of the oxidation/ reduction peaks (in green, Scheme 8, top) compared to ferrocene-free ionic liquids (in orange, Scheme 8, top) are observed, fully consistent with Nernstian diffusion of the redox species within the modified SURGELs. This unexpected finding opens the way to the use of PSM to finely tune the permeability of the amorphous SURGEL coatings.



Scheme 8. Top. Cyclic voltamograms of SURGEL after PSM in neat supporting electrolyte solution (orange) and in the presence of ferrocene in the supporting electrolyte solution. Bottom. Schematics of the increased permeability of the SURGEL after PSM. Adapted from reference 10.

3. Investigation by means of cyclic voltammetry of the film quality of purely organic membranes.

Purely organic films used as membranes have been investigated by means of the set-up described previously and their quality has been demonstrated.[11] The cyclic voltamogram (CV) was recorded using the home build electrochemical cell, where the POF substrate was used as working electrode. The ionic liquid [BMIM][NTf2] (with 4% ethanol) was used as supporting electrolyte and ferrocene (2.85 mM) as electroactive species.

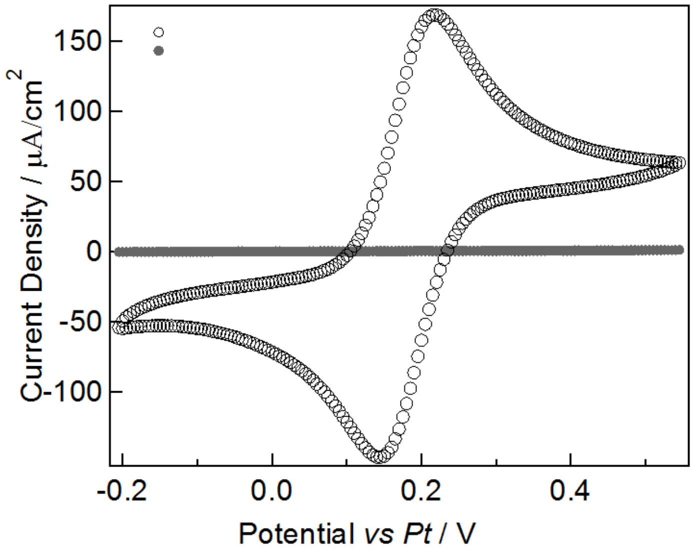


Figure 2. White dot: CV of the SAM used as anchoring layer for the POF. Grey dot: CV of the POF membrane. Scan rate: 0.1 V/s. Platinum wires were used as reference and counter electrode. Adapted from reference 11.

4. Integration of a representative crystalline and porous metal-organic framework - obtained as surface anchored oriented and crystalline films (SURMOFs) of variable thicknesses by means of the stepwise liquid phase epitaxy - in mercury tunneling junctions and the measurements of their electric transport properties.

The fellow demonstrated that the **deposition by evaporation or sputtering** of a metal thin layer film as top electrode is **not** a **suitable** way to achieve the measurement of the vertical conductivity and of the overall electric properties of **SURMOFs**.

Therefore, she worked on an alternative set-up, based on the use of a **drop of liquid mercury (Hg)**: In this case, a drop of liquid and highly conductive Hg is gently deposited on top of the SURMOF, grown on a conductive substrate in order to build a so-called tunneling junction.[14]

Since the results of this work are under review from referees at the time of the submission of this report, they are not included in this publishable summary and are instead described in the periodic report.

4. Impact of the MOLSURMOF project

*Contribution to European excellence and competitiveness.*The use of SURMOFs and MOL-SURMOFs that can be **themselves** used as **robust solid electrodes** has been herein demonstrated to be a successful solution to measure their electrical properties and towards the elucidation of the charge transport mechanism. The **use of SURMOFs** and their **loading with electroactive molecules** has therefore contributed to establish a **completely new field of applications** for these materials. To the best of our knowledge this is the first study of its kind and we believe it will substantially promote the understanding of electric transport properties of MOFs. The knowledge of the factors influencing the charge transport mechanism in SURMOF films, both as pristine and after incorporation of a guest molecule, paves the way towards the exploitation of their predicted and foreseen large potential for applications in electronic devices. The thorough investigation carried out in the frame of this Marie Curie project on the electric transport properties of SURMOFs of paramount relevance both from a fundamental perspective as well as with regards to possible future applications in electronic devices and of the great interest for the whole scientific community. The manuscripts (both published and submitted) place the fellow at the forefront of the investigation in the field, otherwise mainly dominated by research groups established in the USA.[5,6b,7-8]

Contribution to the fellow's training and career development. By the accomplishment of the objectives of the MOL-SURMOF project the fellow got a **daily training** that allowed her to **acquire expertise in a new and emerging field**, as well as to **consolidate her scientific background**. By personally carrying out the laboratory work involved in the MOL-SURMOF project, she gained expertise in several different fields, ranging from the preparation of surface anchored MOF to their characterization by means of many routine and advanced surface characterization techniques, such as X-ray diffraction, infrared reflection absorption spectroscopy and Raman, to name just a few. She was able to **quickly learn new methods** for the electrochemical investigation of thin films, becoming an expert in the field.

Thanks to the **received training**, she will have the **chance to work in any other European research group**, where she will make good use of the gained expertise and work as **tenured post-doc or group leader**, positions not achievable before the granting of the Marie Curie fellowship.

Benefit of the mobility inside the ERA. First of all, thanks to the mobility from Spain to **Germany**, where the fellow could work in one of the leading groups in the field of SURMOFs, the grantee could start **new co-operations** and hence **further enlarge the net of her collaborators**, this being an **excellent basis for the establishment of the own position** in a near future.

Secondly, she had the opportunity to participate in a specific **Mentoring –Training and Networking Program (Tandem Plus)**, jointly organized by the KIT, the Universities of Aachen and Jülich and aimed at **female investigators residing in Germany** who want to know more about the possibilities offered to them in both the academic and industrial sector.

Additionally, she had the unique chance to **further improve** her **knowledge of German**. This is expected to have a huge impact on the further development of her career. In fact, she could not only **opt for** international academic positions where the main language is English, rather also for **German professorship programs**, where an excellent mastery of German is required, **or** for positions as Application Scientist in **German R&D companies**.

Impact of the outreach activities carried out along the 24 months' project. The fellow got involved in **divulgating activities**, these referring both to teaching activities as well as presenting the possibilities offered by the Marie Curie programs.

She took actively part as **teacher** in the ***Thin Films workshop*** organized by her host group in July 2012-2014. She was responsible to teach the participants (Ph.D. students and post-doctoral fellows), the basics of Quartz Crystal Microbalance with Dissipation Monitoring (QCM-D) and Surface Plasmon Resonance (SPR).

Thanks to her **communication skills** together with her truly international experience, and being the first and only Marie Curie IEF fellow at her host institution, she was asked by the organizers of the internal Ph.D symposia to talk about the Marie Curie Actions. This talk was scheduled for the 12th of April 2013.

In addition, willing to act as **Marie Curie Ambassador** wide spreading her experience, she contacted the *Kontaktstelle Frauen in die EU-Forschung (FiF) und die Nationale Kontakstelle Mobilität* (Women Contact Point for EU Research (FiF) and the National Contact point for Mobility) to have the chance to share her experience and hence lecture young women about the Marie Curie Actions by means of sharing her experience. This event took place on the 25th of April 2013. In January 2015, she travelled to Portugal where she showed her scientific results but also briefly talked about the unique opportunities offered to Marie Curie fellows.

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a. Use and dissemination of foreground

Section A (public)

- **Template A1: List of all scientific (peer reviewed) publications relating to the foreground of the project.**

TEMPLATE A1: LIST OF SCIENTIFIC (PEER REVIEWED) PUBLICATIONS, STARTING WITH THE MOST IMPORTANT ONES									
NO.	Title	Main author (corresponding author)	Title of the periodical or the series	Number	Publisher	Year of publication	Relevant pages	Permanent identifiers[2] (if available)	Is/Will open access[3] provided to this publication?
1	Electrochemical investigation of covalently post-synthetic modified SURGEL coatings	C. Wöll	Chemical Communications	No 50	RSC	2014	11129-11131	http://pubs.rsc.org/en/content/articlelanding/2014/cc/c4cc03521f#!divAbstract	no
2	Preparation of Freestanding Conjugated Microporous Polymer Nanomembranes for Gas Separation	C. Wöll	Chemistry of Materials	No 26	ACS	2014	7189–7193	http://pubs.acs.org/doi/abs/10.1021/cm503924h	no

[2] A permanent identifier should be a persistent link to the published version full text if open access or abstract if article is pay per view) or to the final manuscript accepted for publication (link to article in repository).

[3] Open Access is defined as free of charge access for anyone via Internet. Please answer "yes" if the open access to the publication is already established and also if the embargo period for open access is not yet over but you intend to establish open access afterwards.

3	Electric transport properties of surface-anchored metal-organic frameworks and the effect of ferrocene loading	V. Mugnaini, C. Wöll	Applied Interfaces and Materials		ACS	submitted			no

- ***Template A2: List of all dissemination activities***

TEMPLATE A2: LIST OF DISSEMINATION ACTIVITIES								
NO.	Type of activities	Main leader[4]	Title	Date/Period	Place	Type of audience[5]	Size of audience	Countries addressed
1	Poster Contribution to a Conference	The fellow herself	MOF2012, 3rd International Conference on Metal-Organic Frameworks and Open Framework Compounds	October 2012	Edinburgh, Scotland	Scientific Community	>200	-
2	Oral Contribution to a Conference	The fellow herself	113th General Assembly of the German Bunsen Society for Physical Chemistry	May 2014	Hamburg, Germany	Scientific Community	>20	-
3	Oral Contribution to Conference	The fellow herself	ECOSS 30- European Conference in Surface Science	September 2014	Antalya, Turkey	Scientific Community	>40	-
4	Invited Talk	The fellow herself	-	January, 2015	INL, Braga, Portugal	Scientific Community	>20	-
5	Seminar	*The fellow herself*	-	April 2013	IFG/KIT, Germany	Ph.D. Students	>20	-
6	Workshop	*The fellow*		April 2013	Bonn, Germany	Female researchers	>20	-

[4] Intended as the presenter

Section B (Confidential or public: confidential information to be marked clearly)

Part B1

No applications for patents, trademarks, registered designs, etc. were done during the project.

Part B2

Not applicable for an individual MC fellowship.

b. Report on societal implications

A General Information *(completed automatically when **Grant Agreement number** is entered.*	
Grant Agreement Number:	FP7-PEOPLE-IEF: 301110
Title of Project:	MOLSURMOF
Name and Title of Coordinator:	Christof Wöll

B Ethics	
1. Did your project undergo an Ethics Review (and/or Screening)? • If Yes: have you described the progress of compliance with the relevant Ethics Review/Screening Requirements in the frame of the periodic/final project reports? Special Reminder: the progress of compliance with the Ethics Review/Screening Requirements should be described in the Period/Final Project Reports under the Section 3.2.2 *'Work Progress and Achievements'*	***No***
2. Please indicate whether your project involved any of the following issues (tick box) :	
RESEARCH ON HUMANS	
• Did the project involve children?	No
• Did the project involve patients?	No
• Did the project involve persons not able to give consent?	No
• Did the project involve adult healthy volunteers?	No
• Did the project involve Human genetic material?	No
• Did the project involve Human biological samples?	No
• Did the project involve Human data collection?	No
RESEARCH ON HUMAN EMBRYO/FOETUS	
• Did the project involve Human Embryos?	No
• Did the project involve Human Foetal Tissue / Cells?	No
• Did the project involve Human Embryonic Stem Cells (hESCs)?	No
• Did the project on human Embryonic Stem Cells involve cells in culture?	No
• Did the project on human Embryonic Stem Cells involve the derivation of cells from Embryos?	No
PRIVACY	
• Did the project involve processing of genetic information or personal data (eg. health, sexual lifestyle, ethnicity, political opinion, religious or philosophical conviction)?	No
• Did the project involve tracking the location or observation of people?	No
RESEARCH ON ANIMALS	
• Did the project involve research on animals?	No
• Were those animals transgenic small laboratory animals?	No
• Were those animals transgenic farm animals?	No
• Were those animals cloned farm animals?	No
• Were those animals non-human primates?	No
RESEARCH INVOLVING DEVELOPING COUNTRIES	
• Did the project involve the use of local resources (genetic, animal, plant etc)?	**No**
• Was the project of benefit to local community (capacity building, access to healthcare, education etc)?	**No**
DUAL USE	
• Research having direct military use	No
• Research having the potential for terrorist abuse	No

C Workforce Statistics – NOT APPLICABLE, individual fellowship

3. Workforce statistics for the project: Please indicate in the table below the number of people who worked on the project (on a headcount basis).

Type of Position	Number of Women	Number of Men
Scientific Coordinator		
Work package leaders		
Experienced researchers (i.e. PhD holders)		
PhD Students		
Other		

4. How many additional researchers (in companies and universities) were recruited specifically for this project?	
Of which, indicate the number of men:	

D Gender Aspects - NOT APPLICABLE, individual fellowship

5. Did you carry out specific Gender Equality Actions under the project?

○ Yes
○ No

6. Which of the following actions did you carry out and how effective were they?

	Not at all effective				Very effective
❑ Design and implement an equal opportunity policy	○	○	○	○	○
❑ Set targets to achieve a gender balance in the workforce	○	○	○	○	○
❑ Organise conferences and workshops on gender	○	○	○	○	○
❑ Actions to improve work-life balance	○	○	○	○	○

○ Other:

7. Was there a gender dimension associated with the research content – i.e. wherever people were the focus of the research as, for example, consumers, users, patients or in trials, was the issue of gender considered and addressed?

○ Yes- please specify

○ No

E Synergies with Science Education

8. Did your project involve working with students and/or school pupils (e.g. open days, participation in science festivals and events, prizes/competitions or joint projects)?

○ Yes- please specify

X No

9. Did the project generate any science education material (e.g. kits, websites, explanatory booklets, DVDs)?

○ Yes- please specify

X No

F Interdisciplinarity

10. Which disciplines (see list below) are involved in your project?

○ Main discipline[6]: 1.3
○ Associated discipline[6]: 1.2 ○ Associated discipline[6]:

G Engaging with Civil society and policy makers

11a Did your project engage with societal actors beyond the research community? *(if 'No', go to Question 14)*

○ Yes
X No

11b If yes, did you engage with citizens (citizens' panels / juries) or organised civil society (NGOs, patients' groups etc.)?

○ No
○ Yes- in determining what research should be performed
○ Yes - in implementing the research
○ Yes, in communicating /disseminating / using the results of the project

[6] Insert number from list below (Frascati Manual).

11c In doing so, did your project involve actors whose role is mainly to organise the dialogue with citizens and organised civil society (e.g. professional mediator; communication company, science museums)?	○ ○	Yes No

12. Did you engage with government / public bodies or policy makers (including international organisations)

- ○ No
- ○ Yes- in framing the research agenda
- ○ Yes - in implementing the research agenda
- ○ Yes, in communicating /disseminating / using the results of the project

13a Will the project generate outputs (expertise or scientific advice) which could be used by policy makers?

- ○ Yes – as a **primary** objective (please indicate areas below- multiple answers possible)
- ○ Yes – as a **secondary** objective (please indicate areas below - multiple answer possible)
- ○ No

13b If Yes, in which fields?

Agriculture Audiovisual and Media Budget Competition Consumers Culture Customs Development Economic and Monetary Affairs Education, Training, Youth Employment and Social Affairs		Energy Enlargement Enterprise Environment External Relations External Trade Fisheries and Maritime Affairs Food Safety Foreign and Security Policy Fraud Humanitarian aid		Human rights Information Society Institutional affairs Internal Market Justice, freedom and security Public Health Regional Policy Research and Innovation Space Taxation Transport	

13c If Yes, at which level?

- ○ Local / regional levels
- ○ National level
- ○ European level
- ○ International level

H Use and dissemination

14. How many Articles were published/accepted for publication in peer-reviewed journals?	**2**
To how many of these is open access[7] provided?	**0**
How many of these are published in open access journals?	**0**
How many of these are published in open repositories?	**2**
To how many of these is open access not provided?	**2**
Please check all applicable reasons for not providing open access:	
❑ publisher's licensing agreement would not permit publishing in a repository ❑ no suitable repository available x no suitable open access journal available ❑ no funds available to publish in an open access journal ❑ lack of time and resources ❑ lack of information on open access ❑ other[8]: ……………	
15. How many new patent applications ('priority filings') have been made? *("Technologically unique": multiple applications for the same invention in different jurisdictions should be counted as just one application of grant).*	**0**

16. Indicate how many of the following Intellectual Property Rights were applied for (give number in each box).	Trademark	**0**
	Registered design	**0**
	Other	**0**

17. How many spin-off companies were created / are planned as a direct result of the project?	**0**
Indicate the approximate number of additional jobs in these companies:	

18. Please indicate whether your project has a potential impact on employment, in comparison with the situation before your project:

❑	Increase in employment, or	❑	In small & medium-sized enterprises
❑	Safeguard employment, or	❑	In large companies
❑	Decrease in employment,	X	None of the above / not relevant to the project
❑	Difficult to estimate / not possible to quantify		

19. For your project partnership please estimate the employment effect resulting directly from your participation in Full Time Equivalent (*FTE = one person working fulltime for a year*) jobs:	*Indicate figure:*

[7] Open Access is defined as free of charge access for anyone via Internet.
[8] For instance: classification for security project.

Difficult to estimate / not possible to quantify	X

I	**Media and Communication to the general public**
20.	**As part of the project, were any of the beneficiaries professionals in communication or media relations?** ○ Yes X No
21.	**As part of the project, have any beneficiaries received professional media / communication training / advice to improve communication with the general public?** ○ Yes X No
22	**Which of the following have been used to communicate information about your project to the general public, or have resulted from your project?**

❑	Press Release	❑	Coverage in specialist press
❑	Media briefing	❑	Coverage in general (non-specialist) press
❑	TV coverage / report	❑	Coverage in national press
❑	Radio coverage / report	❑	Coverage in international press
❑	Brochures /posters / flyers	❑	Website for the general public / internet
❑	DVD /Film /Multimedia	❑	Event targeting general public (festival, conference, exhibition, science café)

23	**In which languages are the information products for the general public produced?**

❑	Language of the coordinator	❑	English
❑	Other language(s)		

***Question F-10*:** Classification of Scientific Disciplines according to the Frascati Manual 2002 (Proposed Standard Practice for Surveys on Research and Experimental Development, OECD 2002):

FIELDS OF SCIENCE AND TECHNOLOGY

1. NATURAL SCIENCES

1.1 Mathematics and computer sciences [mathematics and other allied fields: computer sciences and other allied subjects (software development only; hardware development should be classified in the engineering fields)]

1.2 Physical sciences (astronomy and space sciences, physics and other allied subjects)

1.3 Chemical sciences (chemistry, other allied subjects)

1.4 Earth and related environmental sciences (geology, geophysics, mineralogy, physical geography and other geosciences, meteorology and other atmospheric sciences including climatic research, oceanography, vulcanology, palaeoecology, other allied sciences)

1.5 Biological sciences (biology, botany, bacteriology, microbiology, zoology, entomology, genetics, biochemistry, biophysics, other allied sciences, excluding clinical and veterinary sciences)

2 ENGINEERING AND TECHNOLOGY

2.1 Civil engineering (architecture engineering, building science and engineering, construction engineering, municipal and structural engineering and other allied subjects)

2.2 Electrical engineering, electronics [electrical engineering, electronics, communication engineering and systems, computer engineering (hardware only) and other allied subjects]

2.3. Other engineering sciences (such as chemical, aeronautical and space, mechanical, metallurgical and materials engineering, and their specialised subdivisions; forest products; applied sciences such as geodesy, industrial chemistry, etc.; the science and technology of food production; specialised technologies of interdisciplinary fields, e.g. systems analysis, metallurgy, mining, textile technology and other applied subjects)

3. MEDICAL SCIENCES

3.1 Basic medicine (anatomy, cytology, physiology, genetics, pharmacy, pharmacology, toxicology, immunology and immunohaematology, clinical chemistry, clinical microbiology, pathology)

3.2 Clinical medicine (anaesthesiology, paediatrics, obstetrics and gynaecology, internal medicine, surgery, dentistry, neurology, psychiatry, radiology, therapeutics, otorhinolaryngology, ophthalmology)

3.3 Health sciences (public health services, social medicine, hygiene, nursing, epidemiology)

4. AGRICULTURAL SCIENCES

4.1 Agriculture, forestry, fisheries and allied sciences (agronomy, animal husbandry, fisheries, forestry, horticulture, other allied subjects)

4.2 Veterinary medicine

5. SOCIAL SCIENCES

5.1 Psychology

5.2 Economics

5.3 Educational sciences (education and training and other allied subjects)

5.4 Other social sciences [anthropology (social and cultural) and ethnology, demography, geography (human, economic and social), town and country planning, management, law, linguistics, political sciences, sociology, organisation and methods, miscellaneous social sciences and interdisciplinary , methodological and historical S1T activities relating to subjects in this group. Physical anthropology, physical geography and psychophysiology should normally be classified with the natural sciences].

6. HUMANITIES

6.1 History (history, prehistory and history, together with auxiliary historical disciplines such as archaeology, numismatics, palaeography, genealogy, etc.)

6.2 Languages and literature (ancient and modern)

6.3 Other humanities [philosophy (including the history of science and technology) arts, history of art, art criticism, painting, sculpture, musicology, dramatic art excluding artistic "research" of any kind, religion, theology, other fields and subjects pertaining to the humanities, methodological, historical and other S1T activities relating to the subjects in this group]