

# SCM - LCF - LPS - Service de chimie moléculaire Rapport Hcéres

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# agence d'évaluation de la recherche et de l'enseignement supérieur

Section des Unités de recherche

# **Evaluation report**

## Research unit:

Service de Chimie Moléculaire (SCM):

- Laboratoire Interdisciplinaire sur l'Organisation
  Nanométrique et Supramoléculaire (LIONS),
- Laboratoire Claude Fréjacques (LCF),

Laboratoire Pierre Süe (LPS).

CEA



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CEA

Le Président de l'AERES Jean-François Dhainaut

Section des unités de recherche

Le Directeur

Pierre Glorieux



# Evaluation report

#### The research unit:

Name of the research unit:

Service de Chimie Moléculaire (SCM),

Laboratoire Pierre Süe (LPS), UMR 9956

Requested label: new UMR CNRS-CEA

N° in case of renewal: fusion of UMR 9956, URA 331 & LIONS

Head of the research unit: Mr Eric ELIOT

### University or school:

CEA

# Other institutions and research organization:

**CNRS** 

## Date(s) of the visit:

March 11-12, 2009



# Members of the visiting committee)

#### Chairman of the commitee:

Mr Francis MAURY, ENSIACET, Toulouse

#### Other committee members:

Mrs Polly L. ARNOLD, University of Edinburgh, Royaume-Uni

Mr Matthias BALLAUFF, University of Bayreuth, Allemagne

Mr Etienne DELOULE, CNRS, Nancy

Mr Lyndon EMSLEY, ENS, Lyon

Mr Claudio LUCHINAT, Unversity of Florence, Italie

Mr Jacques MARTINO, IN2P3, Nancy

Mr Bela MULDER, Fondation FOM AMOLF, Pays-Bas

Mr James F. WISHART, Brookhaven National Laboratory, USA

# CNU, CoNRS, CSS INSERM, représentant INRA, INRIA, IRD...) representatives :

Mr Pierre LABBE, CNU

Mr Jean Marc PLANEIX, CoCNRS





## AERES scientific representative:

Mr Max MALACRIA

Mr Jean-Michel ROBBE

# Research organization representative (s):

Mr Jean-paul VISTICOT, Direction des sciences de la matière, CEA

Mr Remi MICHEL, Direction des programmes, CEA

Mr Francis SECHERESSE, CNRS



# Evaluation report

#### Short presentation of the research unit

- Numbers of lab members: total = 74, including 41 permanent researchers (34 CEA, 7 CNRS), 18 permanent ITA (10 CEA, 8 CNRS) and 15 PhD.
- Numbers of HDR and of HDR who are PhD student advisors: 18 when the form was submitted; 22 at present.
- Numbers of PhD students who have obtained their PhD and average length of a PhD during the past 4 years: 21. Average length of the theses 39 months: they are longer in LPS (40.5 months) than SCM (36.25 months).
- Numbers of PhD students currently present in the research unit: 15
- Numbers of PhD students with fellowships: 15
- Numbers of lab members who have been granted a PEDR: 0
- Numbers of "publishing" lab members: 35

## 2 • Preparation and execution of the visit

The visiting committee was held over 2 days to examine the creation of a new UMR resulting from the merger of a UMR, a URA and another laboratory of the CEA Saclay (hereafter termed the 'fusion project'). The atmosphere of the visit was just right, serious but informal, and everybody felt at ease (both the panel and the groups being evaluated). The organization of the visit was very good, both in terms of logistics and of their enthusiasm with which the researchers described their organization and communicated their results. The schedule was previously prepared with the future director in such a way that the oral presentations of the research were given priority.

The first morning was dedicated to the presentation of the project by its future director and meeting with the scientific council and the representatives of the organisation. In the afternoon, the full committee attended the oral presentations by leaders of all the teams of the "Service de Chimie Moléculaire (SCM)", i.e. LCCEf, LRad, LSDRM and LIONS. The first day provided a good overview of SCM as it ended with a visit of SCM laboratories and a meeting with researchers at a poster session highlighting again the most significant results.

The second morning was devoted to the scientific activity of the "Laboratoire Pierre Süe (LPS)" which was presented by the leaders of the teams, namely GAEL, GTHE, GST, LAPA and LEEL. A meeting with the PhD students of all units (SCM and LPS) and with the laboratory council took place before the visit of the LPS laboratories which included a second poster session. Then the committee met in private to deliberate. Schedules were generally respected.



Nearly half of the committee members are foreigners, and they were pleased that almost all the evaluation was carried out in English. Each presenter provided a copy of his or her slides in English which provided a good summary of the achievements of the team. The quality of documents provided in advance (progress report, project and excel spreadsheets) was satisfactory, but some members suggested that, in line with many research outputs, the use of English as the primary language would enhance the international recognition of the laboratories' research and ensure widespread understanding. On the whole, the presentations of the team leaders closely followed the results presented in the written report. The evaluation team would have appreciated a more careful self-evaluation of their positioning in national and international context, as well as their perspectives and prospective.

The visiting committee appreciated the good organization during the visit from the management team and all staff.

### Overall appreciation of the activity of the research unit, of its links with local, national and international partners

This is a project of fusion of the « Laboratoire Pierre Sue (LPS) », UMR 9956, and the « Service de Chimie Moléculaire (SCM) », consisting of "Laboratoire Claude Fréjacques » (URA 331) and « Laboratoire Interdisciplinaire sur l'Organisation Nanométrique et Supramoléculaire » (LIONS). All these labs are located at the CEA center in Saclay.

The main objective is to achieve synergies for improved efficiency and increased visibility based on complementarities, a larger pooling of resources, a balancing of the ratio researchers/ITA, and refocusing scientific activities on three main axes: (i) materials for energy and environment, (ii) nanosciences, (iii) basic research on nuclear power, while maintaining new technological developments on existing platforms. These scientific topics are well consistent with the scientific policy of CEA and CNRS. This UMR will depend on the Chemistry Department (main) and MPPU Department of CNRS (section 11, 13, 14 and 15).

As a result of this new structure, the "Groupe Science de la Terre" (GST) will move in 2010 from Saclay to the "Institut de Physique du Globe de Paris" (IPGP) and two other groups will disappear because of their subcritical size: "Groupe Toxicité Humaine et Environnementale" (GTHE) and "Groupe Analyse Elémentaire" (GAEL), whose members join the teams LSDRM and LIONS-LEEL, respectively. Apart from some concerns raised by ITA CNRS staff of LPS (the entity most affected), the entire staff appears to subscribe to this new organization.

Having focused on the project in this report, only seven teams were assessed, the six of the new unit and the one that will move: LAPA, LEEL, GST (past activity only), LIONS, LCCEf, LRad and LSDRM.

A common denominator to all labs (both LPS and SCM) is a strong focus on method and instrument development. This feature is a very positive asset but also a potential weakness, as not all the research topics cultivated are up to the standard of the technical skills of the researchers in terms of breadth, general interest and external visibility. The new structure takes this into account and, in agreement with the previous evaluation, this new organization aims to enable the development of individual new research projects by teams that historically were built around specific techniques used principally for service activities.

The overall scientific quality is good but the level of recognition of teams is uneven. The new structure could be addressed though some careful management will be necessary to ensure that smaller teams are not forced into a less promising future because of their small size. The visibility of the scientific output could improve considerably if a more critical self-assessment of the impact of the research topics was used to contribute to an evolution of the overall research strategy. Encouraging signals are already apparent in some of the teams, and this trend should become more general.



The number of publications per permanent research staff member is not very high overall (2.9 papers/researcher.year). The lack of faculty staff and strong link with a university is a disability that results in a relatively low flow of PhD students (approximately 5 theses/year for 18 HDR). Overall the ratio non-permanent to permanent research staff is well below 1, while it is at least 2 in very productive research environments. Recruiting young students and postdoctors is also a matter of attractiveness. In turn, attractiveness depends on quality of research (which is good) but also on visibility (which is less good). Nowadays, a fairly large number of PhD students and postdocs in Europe are not from the same country of the lab they work in. Surprisingly, in this institution the large majority of the non-permanent research staff are French. This could be taken as a sign of lack of sufficient international visibility. This analysis is corroborated by the observation that participation at international meetings by both permanent and non-permanent researchers is, on average, scarce.

On the whole the international collaborations are limited and the committee would welcome a strong strategy to improve this. Furthermore, the positioning of the unit in the major national networks recently established (RTRA, Pole of competitiveness, Carnot network...) has not been presented clearly. The fusion appears as a necessity and the proposers have done a very good job in exploiting this necessity to try and rationalize the research teams and the research strategy in general. They should be congratulated on this. This fusion now provides a good opportunity to rethink some of the research strategies to better exploit the excellent technical competences of the researchers. The committee's overall appreciation of the activity is very positive.

# 4 • Specific appreciation team by team and/or project by project

#### LABORATOIRE PIERRE SÜE (LPS) - UMR 9956

#### 1. Groupe d'Archéomatériaux et Prévision de l'Altération (GAPA)

The "Groupe d'Archéomatériaux et Prévision de l'Altération" (GAPA) was formed in 2006 and it will be renamed Laboratory (LAPA) in the new structure with the same perimeter. This group is very small since it is composed of only 3 researchers (2 CNRS from section 32 and 1 CEA) assisted by a CNRS engineer. However LAPA is also part of a "Laboratoire de Recherche Correspondant" of CEA (LRC DSM01-27) with IRAMAT (UMR 5060 CNRS), which allows sharing of staff and equipments for a better synergy in their field.

LAPA is expert on the study of the evolution of complex metallic systems on very long periods. They develop two research axes and good technical skills in photonic microprobe analysis, especially in the coupling of different micro-beam techniques.

In the first axis, archaeological objects are selected as analogues to predict the long term corrosion and alteration of ferrous materials used in the storage of nuclear wastes and in heritage monuments. The study of the behaviour of multi-barrier systems glass-iron-clay appears as a strategic topic which must be pursued as a priority. This work has implications also in the conservation and restoring of heritage. The second axis addresses the archaeometry with the goal to improve the knowledge on ancient metallurgical processes. Both axes require a multi-scale approach and a good expertise in advanced analytical techniques as  $\mu$ XRD,  $\mu$ XRF, nuclear  $\mu$ probe, photonic  $\mu$ probe and  $\mu$ XAS on synchrotron beam lines, and LAPA has a specific position in archaeometry due to is strong analytical expertise.

The 2 axes will be carried on in the future unit where LAPA will contribute essentially to one of the three general topics: the nuclear field. Perspectives are quite good since they will benefit from new equipments as MICROSCOPIUM beam line at synchrotron SOLEIL for which they were involved in the design. Their project to strengthen their collaboration with the LEEL group for the detection of light isotopic elements by nuclear microprobe is encouraged.



#### – Strong points:

- Great expertise in chemical and structural analysis of complex materials using micro-beam techniques.
- The implementation methodology on archaeological analogues is innovative: multi-devices and multi-scale characterization, specific tests to valid the hypothetical mechanisms and modeling to predict the lifetime.
- Restoring corrosion of samples in isotopically marked media is an original approach to study the corrosion mechanisms.
- Good productivity (2.2 papers/researcher.year).
- The development of the photonics platform is an asset for the entire unit.

#### — Weak points:

- The small size of the team limits its visibility and recognition.
- Publications in international peer-reviewed journals with greater impact than national journals must be preferred.

#### Recommendations:

- Efforts should be made to strengthen national and international collaborations.
- The studies on archaeometry contribute to the basic knowledge and to the development of analytical tools but, due to the small size of the group, this activity should not consume too many resources to the detriment of the 1<sup>st</sup> axis which should be a priority.

An engineer position is recommended to support the development of the photonics platform, especially coupling between the various techniques which will be useful for the entire Unit.

Nom de l'équipe : Groupe d'Archéomatériaux et Prévision de l'Altération (GAPA)

Note de l'équipe	Qualité scientifique et production	Rayonnement et attractivité, intégration dans l'environnement	Stratégie, gouvernance et vie du laboratoire	Appréciation du projet
В	А	В	В	В

#### 2. Laboratoire d'Etude des Eléments Légers (LEEL); replacing Groupe Microsonde Nucléaire (GMN)

The LEEL is replacing the "Groupe Microsonde Nucléaire (GMN)" from the LPS during the previous period. For the 2004-2007 period, the beam time of the nuclear microprobe was devoted about 60 % to the GMN, and 40 % to external users, allowing completion of 18 different external projects each year, the nuclear microprobe being in use 2400 h/year. This beam time distribution is a major change compared to the 2000-2004 period, when 80 % of the beam time was devoted to external users.

The GMN is composed of only 3 researchers (2 CEA and 1 CNRS from section 15) assisted by 5 ITA. Another ITA engineer from GAEL will join to form the new LEEL group.

The scientific activity of the GMN was mainly focuses on the behavior of materials for nuclear energy (hydrogen transport in ceramic membranes, hydrogen and helium distribution in nuclear fuel cladding tubes, or He diffusion in irradiated  $UO_2$ - $PuO_2$ ), the irradiation effects on cells with the development of the single-ion experiments, and on support to Planetary and Earth Sciences, with the connection to the NASA Stardust mission for comet coma grain analysis and water content determination in nominally anhydrous minerals (microERDA development).



The GMN scientific production is attested by the publication of 38 papers in international journals, mainly related to nuclear physics. The main focus of the team on subjects linked to nuclear energy materials implies a restricted field of collaboration and a restricted audience, without any negative implications towards the high quality of the experiments and technical developments.

The long-term goal to overhaul the microprobe accelerator represents an important commitment to the future development of this group, its own research program, and the collaborations with other labs within this organization and externally. Increasing demand for the instrument can be addressed through efficiencies obtained via performance improvements, automation, and making the machine easier to use. They are important for relieving the stress caused by increasing internal research activities while maintaining an acceptable level of availability for outside users as described above.

#### — Strong points:

The main instrumental developments for the 2004-2008 period are the single ion setup for low dose irradiation, an enhanced ERDA setup and pp scattering (ERCS) for the hydrogen detection. These developments are impressive and they will enable a wide range of future scientific investigations, allowing LEEL to be one of the best groups in the world for light element analysis and for studies of physical radiobiology through the ability to target specific structures in the cell.

#### — Weak points:

 Even if the GMN seems to be involved in international collaboration and accustomed to participation in international meetings and workshops, the participation in international meetings is focused on a restricted field, and the teaching activity, as well as the diffusion of knowledge, seems to be limited, and all confined to France.

#### Recommendations:

- We should note that one researcher has left the group without being replaced up to this point. We support the stated intention to reinforce the staffing of the lab with the CR request to the CNRS to replace the departure and the CEA researcher position to study the behavior of gases in nuclear materials. These appointments will augment the nearly completed historical transition of this group from a technique-based service to a research entity with specialized expertise of value to many fields.
- In the new Unit LEEL will be in close association with several other groups, such as LAPA, LRAD and LSDRM. The efficiency of the group to provide high quality results on its own time could support this repartition of machine time. However, the allocation of beam time to external scientists is also an opportunity for LEEL to develop new scientific collaborations, and to motivate progress on both the instrumental and scientific fronts. Furthermore, the nuclear microprobe is a national instrumental resource, with specific development. Therefore access for external scientists should be preserved, with national calls to provide the best scientific projects with access to this device. This should be a good way to develop the international visibility of the laboratory.

Nom de l'équipe : Laboratoire d'Etude des Eléments Légers (LEEL)

Note de l'équipe	Qualité scientifique et production	Rayonnement et attractivité, intégration dans l'environnement	Stratégie, gouvernance et vie du laboratoire	Appréciation du projet
В	А	В	В	А



#### 3. Groupe Science de la Terre (GST)

The "Groupe Science de la Terre (GST)" has a special activity in the Pierre Sue Laboratory, because this group as the GAPA is devoted to a scientific thematic and not to the development of a specific instrument and method. The GST group is a relatively small group at the national or international scale (6 permanent peoples, when including a researcher retired in 2008).

The activity of the group is focused on the study of the mechanisms and budgets of magmatic fluid transfer, with 5 main directions: (i) gas emissions and eruptive dynamisms, (ii) volatiles in magmas and degassing mechanisms, (iii) magma geochemistry via trace elements in melt inclusions, (iv) trace elements geochemistry by INAA, and (v) experimental approach of mantle and magmatic fluids.

The publication rate of this group is very good, with 51 publications in international peer-reviewed journals, with several papers in high impact factor journals (Nature, Science, Geology), with more than two papers published each year by 5 scientists on 6 in the group. Over the 4 years, the group also demonstrated a good capacity to establish national and international collaborations: the 56 published articles pointed out the active participation of 11 different scientists, almost twice the group size. The group has a strong international activity, with 75 communications in international meetings, the organization of IUGC, EGU and AGU sessions, and the writing of 3 chapters in the Stromboli AGU monograph. 4 PhD theses were performed during this period. The PhD students benefit from a good support from the group, with a large access to the instruments and to the international workshop and meeting. The GST gives the needed support to its younger member to develop her own research axis and a PhD student grant. The move to IPGP confirms the good scientific quality of GST.

#### — Strong points:

- The group has developed a very good expertise in several different techniques, nuclear microprobe and INAA, the specific Pierre Sue Laboratory tools, but also gas mass spectrometry, μRaman, μFTIR and Xray spectroscopy, OP-FTIR and UV absorption spectrometry.
- Strong international collaborations.

#### – Weak points:

The weakness of this group may be in the future the absence of young researcher, since the youngest one moved for the IMPM in 2008. However the displacement of this group from the Pierre Sue Laboratory toward the "Institut de Physique du Globe de Paris (IPGP)" and University Paris 6 should allow a better attractiveness for students and young researchers.

#### Recommendations:

- No comment on the project of this group since it is moving to IPGP.

Nom de l'équipe : Groupe Science de la Terre (GST)

Note de l'équipe	Qualité scientifique et production	Rayonnement et attractivité, intégration dans l'environnement	Stratégie, gouvernance et vie du laboratoire	Appréciation du projet
A+	A+	A+	А	Non noté



#### SERVICE DE CHIMIE MOLECULAIRE (SCM)

#### 1. Laboratoire Interdisciplinaire sur l'Organisation Nanométrique et Supramoléculaire (LIONS)

The LIONS appears as a dynamic laboratory which has largely achieved the objectives set in 2004: creating an effective unit in basic research on the topic of nanosciences related to the self-assembly.

It is composed of 13 permanent researchers from CEA. Their multidisciplinary expertise and their ability to develop a strong symbiosis between statistical physics and advanced physico-chemical characterization combined with high-tech instrumental developments is a strong feature of this laboratory.

The scientific activity and the organization are not based on research teams but are rather carried on under projects. This organization is effective since the scientific production is quite good (102 publications in international journals, 31 invited lectures). They got good success to calls for proposals (ANR, C'Nano, RTRA, Europe) and have committed many collaborations either in France or abroad. The laboratory is also strongly involved in the missions of research training (doctorate school and PhD students), teaching (master level) and expertise.

The project for 2008-2011 aims the realization of materials and innovative devices by self assembly with applications consistent with the main objectives of the CEA, *i.e.* the field of information, energy or health. This project is based on a strong coupling between theoretical studies, basic research and technical skills for the instrumental developments such as coupling of major instruments with micro- and nano-fluidics. The LIONS includes a recruitment policy with a strategy for research funding to carry on projects not yet supported by ANR.

#### — Strong points:

The visiting committee was impressed by the quality of individual researchers of LIONS. It was also pleased by the ability of the laboratory to participate in missions of research training and formation of many PhD students.

#### — Weak points:

- Most of the research projects themselves are interesting. It appears, however, difficult to identify "the visible image" of this laboratory. Similarly, regarding the number of permanent researchers constituting the laboratory, its visibility at the international level should be improved.
- Work on the toxicity of nanoparticles, although certainly important for applications in the current societal context, appears superimposed on the general activities of the laboratory and deserves a strengthening as its own specific area from a scientific point of view.
- The physics of soft condensed matter is traditionally very strongly coupled with the theory and simulation. Despite the presence of two theoretical researchers in the laboratory, it appears important to strengthen this sector to develop in the future work with a greater impact.

#### — Recommendations:

- To improve the visibility of the LIONS for instance through organisation of international conferences, even on the site of Saclay, or by more publication of "reviews" in international journals.
- To strengthen the research potential in the fields of theoretical physics and simulation and to strengthen more scientifically the research on the toxicity of nanoparticles.



Nom de l'équipe : Laboratoire Interdisciplinaire sur l'Organisation Nanométrique et Supramoléculaire (LIONS)

Note de l'équipe	Qualité scientifique et production	Rayonnement et attractivité, intégration dans l'environnement	Stratégie, gouvernance et vie du laboratoire	Appréciation du projet
А	А	В	А	А

#### 2. Laboratoire de Chimie de Coordination des Eléments f (LCCEF)

The LCCEF is a relatively small team (6 permanent researchers) characterized by a very good scientific productivity (5 papers/researcher.year), with a significant portion of the work published in journals with high impact factor.

The research areas are focused on the design and synthesis of new compounds of uranium and rare earths. The general objectives of the work are the preparation of complexes in which metals have unusual oxidation and environments and/or specific chemical or physico-chemical properties.

Although these works are situated in a highly specialized area, the variety of studies and applications covered represent a significant and original scientific contribution recognized by the best journals in chemistry. The developments of these studies in the fields of catalysis and especially of optoelectronic devices are certainly areas to reinforce. For this axis, it also seems important to broaden the issue of basic research at the same time that the work must be developed for compounds currently the most promising. Studies on other bridging and terminal ligands and other polynuclear systems should be conducted in parallel.

#### – Strong points:

The complex chemistry of high oxidation of uranium is undeniably a strong contribution of the group. The activation of the uranyl ion providing an interesting reactivity of this ion is highlighted, in particular to obtain a stable compound of the  $UO_2^+$  ion. The development of uranyl complexes with organic polycarboxylates ligands is a breakthrough: one wonders however what the goals are.

#### — Weak points:

One must regret the cessation of studies on the magnetism of these compounds which could lead to interesting applications since the coupling of two properties seems possible. Indeed, on one hand the synthesis of polynuclear complexes is controlled (particularly with metals with two different degrees of oxidation) and, on the other hand ligands with coordination properties allowing the synthesis of heterometallic polynuclears exist.

#### - Recommendations:

- Theoretical studies and knowledge of the metal-ligand have recently been addressed and should be developed through collaboration with the work on synthesis and study of physico-chemical properties.
- The influence of the group both in the French academic community and abroad could be stronger. A difference exists between the quality of the journals where the results are published and the number of invited lectures.
- Intervention in the teachings of Masters degree programmes should also be significantly higher, which would facilitate recruitment of PhD students or postdocs. Recruiting more diverse, motivated and bright undergraduate and PhD students from universities and schools in chemistry is also necessary for the development of the group.



- Strengthening the team in the context of fusion of the two laboratories should be a priority for balance in the field of synthetic chemistry. Thus, a policy of active recruitment should be initiated quickly: reinforcements in the area of synthesis (new ligands and complexes) and physico-chemical studies of molecular materials appear indispensable, both for the development of the team in the short term and its sustainability over the medium term.
- The team leader will retire in the foreseeable future and to ensure the sustainability of LCCEf his successor must be quickly identified.

Nom de l'équipe : Laboratoire de Chimie de Coordination des Eléments f (LCCEF)

Note de l'équipe	Qualité scientifique et production	Rayonnement et attractivité, intégration dans l'environnement	Stratégie, gouvernance et vie du laboratoire	Appréciation du projet
A	А	В	А	А

#### 3. Laboratoire de Radiolyse (LRad)

The activity of LRad over at least the four past years is excellent. It should be noted that the group is focussing on studies that are relevant to the missions of the CEA and in general to topics related to energy. The evidence for continuity on such a track over the coming years appears very convincing. The group relies on impressive experimental equipment (Alienor and its uniquely specialized experimental set-ups, the gamma irradiator, etc.), partnerships with other facilities (such as GANIL and ELYSE at Univ. Paris XI) and participation in future facilities (like Arronax). The research topics on various facets of water radiolysis (under heavy ion irradiation, supercritical conditions, bound to surfaces, confined spaces, and applied to radical biochemistry), and a recent initiative on organic material radiolysis, can be qualified as dynamic, timely and on the forefront.

#### — Strong Points:

- Towards the end of the period under evaluation there were two departures of senior personnel from this group, however the younger generation has stepped forward with a coherent strategic vision for the future and they have equipped themselves with the necessary experimental tools to accomplish it.
- There is a judicious choice of timely research topics, well focused on certain aspects of water radiolysis (a subject with a long history) that could only be solved with today's equipment and techniques and that are relevant to current problems such as water chemistry in new-generation reactors, radiolytic corrosion (confined spaces), and surface and interior radiation chemistry of waste forms, among others. There are also valuable lines of research with medical and biological implications, including heavy-ion radiotherapy, mechanisms of biomolecule and cell damage, and radioprotectants.
- Despite the group's relatively small size and lack of technical support, they have managed to assemble a remarkable variety of specialized experimental apparatus (SCW, high-pressure, gas sampling, IR detection) to enable their ambitious experimental program, and they wish to add more (EPR).
- The LRad is a top-level group in the field of radiation chemistry within Europe and the rest of the world. Within France its activities are complementary to the ELYSE picosecond pulse radiolysis facility of the Université de Paris 11. The LRad has strategic collaborations with ELYSE and several other laboratories nationally and internationally, including femtosecond IR pulse-probe spectroscopy, and a good record of publication in major journals.



#### – Weak points:

- Theoretical support is very important to understanding the results obtained in this laboratory. There is recognized expertise in molecular dynamics simulations within the group, however mesoscale simulations are important also for the work in confined systems. Perhaps for lack of time, the LRad presentation did not emphasise the existing ANR-supported collaborations with CIMAP and LIRIS on these subjects, which deserve attention.
- The condition of the accelerator and related instrumentation was excellent and a good reflection on the researchers and the technician, however there should be more general technical support so that the group can focus on the science instead of being part-time machinists and electrical engineers.

#### Recommendations:

- To remain on the excellent track followed so far.
- To maintain a strong and visible position in the world radiolysis network through the continued development of advanced instrumentation, cutting-edge research, and strategic national and international collaborations.
- It is strongly recommended to follow through on the intention stated in the recruitment policy of the fusion project document to create a researcher position in the LRad to develop new radiation sources for studying elementary steps in radiolysis.
- To get more technical support for Alienor and instrumental development, including but not limited to the shared IR position mentioned in the recruitment policy.

Nom de l'équipe : Laboratoire de Radiolyse (LRad)

Note de l'équipe	Qualité scientifique et production	Rayonnement et attractivité, intégration dans l'environnement	Stratégie, gouvernance et vie du laboratoire	Appréciation du projet
A+	A+	A+	А	A+

#### 4. Laboratoire de Structure et Dynamique par Résonance Magnétique (LSDRM)

The NMR laboratory (6 permanent researchers) is performing globally very well. They have a broad range of projects, from biosensors in solution, through materials NMR to advanced instrumentation. In some projects they are clearly among the world leaders. In others their contribution is less significant, but is always of a good level, and always among the best in France.

The originality of the research activity is globally high. Most notably, rotating coil magic angle spinning (MACS), and the design of portable magnet systems are particularly innovative ideas, and have the perspective of high impact on a broad community. The interest of the portable magnet systems is especially high, as is the Xenon biosensor work and the work on characterising glasses. Work on tritium, multiple echoes, and noise detection, are all innovative projects, but these will probably have less impact. All the projects in the lab are concerned with cutting edge scientific problems.



There is overall high quality of the scientific papers, with 1 Nature, 3 PNAS, and 5 JACS papers among the 66 papers published in the period since 2004 (roughly 2.5 papers/researcher.year). However, while the MACS work has notably achieved worldwide visibility, the notoriety of the other subjects has so far resulted in significantly less visibility at the international level (while all are well known in the French NMR community). The group should make an effort to be more productive in terms of the volume of publication. They should be present at all the key conferences in their area worldwide. This is currently not the case, and contributes to the work often being globally under-evaluated. This is also reflected in the relatively low level of citations for the historical subjects in the laboratory.

The added value of the research on knowledge or technology is globally high. Their work contributes significantly to knowledge about glass structure, spin dynamics, and NMR instrumentation. Similarly, the intrinsic technical scientific quality of the work is high, which has impact on software for quantifying spectra, instrumentation, and NMR methodology in highly polarised systems.

Management of the team is clearly fairly good, for example in respect to the hiring strategy. Recent recruitments add to the long-term viability and to the credibility of the ongoing projects. There are no major foreseeable problems in this respect. The focus of the group is clearly on development, with three application areas fairly clearly delineated. It may be worth noting that if the group went slightly further towards well chosen applications, the degree of uptake of the methods would certainly be higher, and more rapid, leading to wider notoriety.

Previous goals have been largely achieved. However, very little information is given about perspectives in the report. The Revolution NMR project, as well as the extension of Xe biosensors to animal imaging, are both exciting and ambitious objectives which should be given full support. In particular, these are clearly high-risk projects in front line research. With the available information, it is difficult to evaluate if the other projects (concerning materials, or spin dynamics in polarised gasses) are in continuity or if they propose any breakaway ideas.

#### — Strong points:

- All the work carried out in the lab is of high merit. Special attention should be paid to giving full support to the particularly excellent projects concerned with (i) instrumental development, and (ii) Xenon biosensors. Both projects are highly original and innovative, and have the potential for great broad impact.
- The unit has significant promise in terms of several of its young researchers, as is very strongly highlighted by the award of an ERC starting grant to one of the group members.

#### — Weak points:

- We regret that there is a relatively low number of PhD students. Also, there is little contribution to knowledge dissemination or to scientific culture, to social and scientific interactions.

#### – Recommendations:

- The importance and relevance of scientific cooperations could be increased to a more international level. Notable exceptions are work on portable magnet systems, resulting in part from a strong collaboration with a group in Berkeley, and the work on biosensors, resulting from a strong national collaboration with the ENS-Lyon. In particular, the implication in national and international networks is relatively low.
- Additionally, we believe that industrial partnerships could be fruitfully developed on both biosensors and on magnet systems. The team is in particular highly competent in operational knowledge. However, there is so far little transfer of technology, neither on the instrumentation, nor on the hyperpolarisation or biosensor sides, despite the presence of patents. The impact on society is potentially real, but has not yet been realised. In order for them to make more headway in the biomolecular field they should build up stronger collaborations. Some of the examples they presented (e.g. the work on Taxol) did not seem connected to well-articulated questions from the biological side.



Nom de l'équipe : Laboratoire de Structure et Dynamique par Résonance Magnétique (LSDRM)

Note de l'équipe	Qualité scientifique et production	Rayonnement et attractivité, intégration dans l'environnement	Stratégie, gouvernance et vie du laboratoire	Appréciation du projet
А	А	В	А	А

### 5 • Appreciation of resources and of the life of the research unit

The structuring of the new Unit in 6 teams is consistent with the objectives of better balance and focus on strong topics. However one of the teams (LAPA) retains a very small size hampering its visibility and therefore its sustainability. Reflection on the internal structure should therefore continue. The good complementarity of the teams leads to multiple inter-team collaborations and should enable a greater efficiency in response to calls for proposals. Transverse actions conducted by a project team constituted of members from several groups already exist and are encouraged.

Despite some legitimate concerns as to the restructuring, the staff endorse this project of fusion. The biggest concerns come from ITA CNRS staff that appear to have been less informed and should be reassured. From this point of view the Laboratory Council has a vital role to play: it is a statutory forum where all categories of staff should be represented and whose findings are reported in minutes. A functional organizational chart indicating clearly the responsibilities does not seem to have been distributed to all staff. This requires an immediate action especially as the new structure is already in place.

Dispersed over several buildings on the site of Saclay, the new UMR should avoid a federal operation only based on the founding laboratories. Efficient internal communication and active scientific animation is a key point to do that. The physical location of the research labs is far from a university campus, so the PhD, post-docs and undergraduate students need to feel part of a dynamic scientific community which will give them a sense of belonging to a well-known laboratory rather than an individual team. When they leave they continue to contribute to the influence of the laboratory and this should not be overlooked.

Little information has been communicated on the budget but it appears that the most of funding comes from annual resources of the CEA and CNRS, although external resources tend to increase with the ANR. The new UMR is involved in 14 ANR projects, which are very unevenly distributed among the teams, and those who have attracted ANR funding should be used as good examples to the other research teams. Financial management seems to be centralized; the management team has the means to implement its policy.

The main activity involving nuclear technologies, the aspects of health and safety are fundamental. They have not been addressed during the audit but everyone knows that it is a very important point on the site of Saclay and it is good to see that several safety engineers are an integral and important part of the management team with responsibilities for building.



#### 6 • Recommendations and advice

Some strengths and weaknesses have been reported earlier in this report and we therefore limit ourselves to a few more general comments.

#### — Strong points:

- The main activity of the founding units (LPS and SCM) is to develop fundamental research for nuclear programs and the use of nuclear technology. This project of fusion of the two laboratories is coherent, viable and well conducted. From the historical skills based on method and instrument development, it should allow a better development of cutting edge research which is expected to be at the highest international level because of the quality of equipment available on the site of Saclay and competence of researchers.
- Many instruments developped during the 2004-2008 period are impressive and are important assets for the future: e.g. the single ion setup for low dose irradiation, an enhanced ERDA setup and ERCS for the hydrogen detection, the photonic platform and coupling of various techniques in addition to the historical facilities. This lab has a great expertise in chemical and structural analysis of complex materials and analysis of traces elements.
- Much of the work carried out in the lab is of high merit. The strengths are noted above for each team. Overall the LRad is a top-level group in the field of radiation chemistry within Europe and the rest of the world. Other teams have a favourable environment to achieve the highest levels of recognition.

#### – Weak points:

- The external visibility must be significantly improved. The small size of some team limits their impact and recognition.
- Overall there is little involvement in education. Furthermore there is a relatively low number of PhD and undergraduate students. This is probably due to the lack of faculty staff and strong link with a University. Researchers do little teaching.
- The large majority of the non-permanent research staff are French. The unit is encouraged to recruit some PhD's at the international level.
- The productivity of some groups could be improved, and the participation in international scientific meetings by *both* permanent and non-permanent researchers is, on average, low.
- The contribution to knowledge dissemination or to scientific culture, to social and scientific interactions could be improved.

#### – Recommendations:

- The proposers have done a very good job in exploiting this fusion to rationalize the research teams and the research strategy in general. This is a good opportunity to rethink some of the research strategies to better exploit the high technical competences of the researchers. It seems that the team leaders are not sufficiently involved in this strategy. Once having identified areas of excellence, one must define the fields in which the unit wants to be unavoidable and this cannot be all the areas. A Scientific Council with external and independent renowned scientists may help to define this.
- Efforts should be made to strengthen national and international collaborations. More involvement in national and international networks as well as international meetings are also recommended.



- The nuclear microprobe is a national instrumental resource and access for external scientists should be preserved, for instance with national calls to provide the best scientific projects. This also provides a good way to develop the international visibility of the laboratory.
- Focus on the career development of the future leaders of the teams (and strategic themes) where senior members will retire soon.
- All the stakeholders (CEA, CNRS and lab staff) agreed on a peculiar management scheme with a Lab Head taking care of general management, administration and safety issues, with the help of a good scientific advisory board in charge of scientific strategy and production.
- The laboratory must have a thorough reflection on the training at the doctoral and master level which is the breeding ground for recruitment. The "life" of the lab should be encouraged through a policy of regular seminars, recognized and coordinated with the doctoral school.

Note de l'unité	Qualité scientifique et production	Rayonnement et attractivité, intégration dans l'environnement	Stratégie, gouvernance et vie du laboratoire	Appréciation du projet
A	А	В	А	Α



Monsieur Pierre GLORIEUX Directeur de la section des unités

AERES 20 rue Vivienne 75002 PARIS

Saclay, le 26 mars 2009

**Objet :** Réponse du CEA au rapport d'évaluation du SCM-LPS (Référence : EVAL-0912281K-S2100012505-UR-RPRELIM)

Nos réf.: DPG/AN/np/2009-162

Monsieur le Directeur,

Le Service de Chimie Moléculaire (SCM), unité composée du Laboratoire Claude Fréjacques (URA CEA-CNRS) et du Laboratoire Interdisciplinaire sur l'Organisation Nanométrique et Supramoléculaire, ainsi que le Laboratoire Pierre Süe (LPS, UMR CEA-CNRS) ont été évalués par l'AERES. Le projet de fusion du SCM et du LPS qui, en utilisant les complémentarités de ces unités, a pour but d'accroître l'efficacité de la recherche et sa visibilité ainsi que de rééquilibrer les équipes de recherche, a été jugé positivement par le comité d'évaluation. Le CEA remercie l'AERES et le comité d'évaluation pour son travail d'analyse des activités du SCM et du LPS et va prendre en considération les recommandations du rapport afin d'améliorer encore la qualité de la nouvelle unité.