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## LAMBE - Laboratoire d'analyse et modélisation pour la biologie et l'environnement

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:

Laboratoire d'Analyse et Modélisation

pour la Biologie et l'Environnement (UMR 8587)

Université Evry Val d'Essonne



march 2009



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# Evaluation report

Research unit

Laboratoire d'Analyse et Modélisation

pour la Biologie et l'Environnement

Université Evry Val d'Essonne



Le Président  
de l'AERES

Jean-François Dhainaut

Section des unités  
de recherche

Le Directeur

Pierre Glorieux

march 2009



# Evaluation report



## The research unit :

Name of the research unit : Laboratoire d'Analyse et Modelisation pour la Biologie et l'Environnement

Requested label : UMR

N° in case of renewal : 8587

Head of the research unit : Mme Jeanine TORTAJADA

## University or school :

University Evry Val d'Essonne

## Other institutions and research organization:

CEA Saclay

CNRS

## Date(s) of the visit :

12 février 2009



# Members of the visiting committee

## Chairman of the committee :

M. Detlef SCHROËDER, Institute of Organic Chemistry and Biochemistry, Czech Republic

While the report is written in English, Dr. Schroeder is reasonably fluent in French, led the discussions in French and if any aspects of language or particularities of French administrations would have remained unclear during the evaluation, the other experts of the committee immediately gave comprehensive explanations/clarifications.

## Other committee members :

M. Redouane BORSALI, CERMAV, Grenoble

M. Mark E. CASIDA, Université de Grenoble 1

M. Eric FOREST, Université de Grenoble 1

M. Bernd GRAMBOW, Ecole des Mines de Nantes

M. Stephane HUMBEL, Université Aix-Marseille 3

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

Au titre du CoNRS, Mme Catherine COMBELLAS

Au titre du CNU, M. Serge GERIBALDI



# Observers

## AERES scientific representative:

M. Max MALACRIA

## University or school representative:

M. Richard MESSINA, Président de l'Université Evry Val d'Essonne

## Research organization representative(s) :

M. Francis SECHERESSE, Représentant CNRS

M. Bernard BONIN, Représentant CEA



# Evaluation report

## 1 • Short presentation of the research unit

- Numbers of lab members : 46,5 including 42 researchers with teaching duties and full time researchers (5PR, 1PREM, 18MCF, 6 CNRS, 12 CEA) including 8 PR/DR and 34 MCF/CR, 3,5 engineers, 6 post-docs, 13 doctoral students, 1 administrative assistant ;
- Numbers of HDR : 15 ;
- Numbers of lab members who have been granted a PEDR : 5
- Numbers of “publishing” lab members : 35

## 2 • Preparation and execution of the visit

After having received a detailed and well-prepared dossier (Report 2005-2008, Project 2010-2013, Bibliometric data) as hard copy and - upon request of the president of the committee - comprehensive additional information about the inter-team collaborations in 2005-2008 (joint papers, patents, grants etc.), the members of the committee studied the printed material and were thoroughly prepared for the meeting. The meeting itself took place on Thursday, Feb. 12, 2009, in the rooms of the Université d'Evry. The meeting began at 9 h with a presentation by the director of the UMR 8587 followed by presentations of the leaders of the four research groups defined in the following as Teams 1 - 4. To facilitate drafting the report and concentrate efforts and expertise, the committee formed subpanels of experts for the teams.

Team 1. *Structure-réactivité de biomolécules: Complexes organométalliques et macromoléculaire*

Team 2. *Interactions des assemblages moléculaire complexes: Théorie et modélisation*

Team 3. *Réactivité aux interfaces dans l'environnement*

Team 4. *Matériaux polymères aux interfaces*

At ca. 12.30 h, the presentations were followed by a poster session (with embedded lunch), in which the members of the committee had and used the opportunity to clarify further details with the various teams and also to directly contact selected researchers for discussions of projects and career opportunities. The president also directly offered the availability of all members of the committee for confidential conversations. The poster session (ca. 2 h) was followed by a 30 min. tour through the laboratories of Teams 1 and 4. Afterwards, two separate meetings with the technical personal (ca. 30 min.) and the Ph.D. students / postdocs (ca. 45 min.) were held. After a brief internal coordination, a ca. 45 min. meeting with the President of the Université d'Evry, and several representatives from the related organizations (CEA, CNRS, Génopole, Université de Cergy-Pontoise) concluded the official part of the audit (ca. 18 h).

Due to the early leave of one member of the committee, an initial meeting took place in the rooms of the UMR 8587 (18 - 19 h), followed by dinner and a meeting from 21 h to midnight in which the conceptual evaluation was made. Tuning and finalization of the report took place via email within the week after the visit in Evry.



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

In general terms, the UMR 8587 can be classified as a laboratory from physical chemistry with a strong orientation towards analytical chemistry. While such a formal classification is always simplistic, in the case of the UMR 8587 it is particularly crude because the unit is an example of truly multidisciplinary research. Thus, in addition to the profound expertise of the chemists in all four teams, the UMR 8587 includes physicists, biologists, and experts from the CEA Saclay. This highly interdisciplinary structure is almost unique in France and merits profound support. The gender and age structure of the UMR is very good and promises continuous and successful development in the future.

The suggested development of the UMR 8587 includes a change of the research topics to still even more biologically relevant questions and the committee rates this orientation as very positive. Particular strength to this new direction is given by the anticipated inclusion of the new Team 4; a very productive and internationally recognized group with a highly multidisciplinary character between chemistry, physics, and biology. The development of the other teams is in part oriented towards a continuation of the previous successful lines of research and in equal parts towards new, attractive avenues in chemical sciences.

Concerning visibility, within the report period the UMR has contributed an appreciable number of communications and full papers in well-recognized scientific journals, the members actively participated in many national and international conferences by either lectures or poster presentations, and also submitted several patents. Further remarkable are some publications in high-impact journals (IF > 8; only Teams 1 and 4). While the performance of the separate teams somewhat differs as detailed below, the general appearance is quite good: the national visibility is high and the international visibility clear. Particularly noteworthy in this respect are the participations of the UMR 8587 in missions to European Multi-user facilities such as CLIO and SOLEIL. Further, the activities between the teams are good as far as joint papers and grant applications as well as patents are concerned, although the collaboration of some of the teams might still be strengthened (for details, see comments to the separate teams). While a considerable share of applications to French funding agencies were successful, the number of international grants is limited and no large applications to European funding agencies are currently ongoing; specific engagement in this direction (e.g. ERC grants or training networks) is thus strongly encouraged.

While Team 1 has recently been equipped with a "large machine" (*Orbitrap* mass spectrometer), the overall instrumental equipment would profit from improvements in the future; a specific point would be an NMR spectrometer better than the present 300 MHz for Team 4. An attractive issue is certainly the anticipated acquisition of an ion-mobility mass spectrometer, which offers particularly strong potential in the combination with life sciences.

An important point for a possible improvement concerns the recruiting of Ph.D. students to the lab in Evry, as only 12 Ph.D. theses were finished within the report period (new Team 4 not included). For a group of permanent scientists of the size of UMR 8587, an increased number of Ph.D. students certainly is desirable, and the UMR as well as the University itself (perhaps with assistance by the Genopole) should consider this aspect as an important point on the future agenda. Related with this point, the leadership of the UMR 8587 as well as the administration of the Université d'Evry might consider means to identify and then support particularly excellent scientists. A possible concrete example in this respect would be the reduction of the teaching load of those young scientists in the teams which have potential for scientific excellence (e.g. CNRS delegations or ANR grants). A second critical issue deals with the intergroup relationships which certainly can be improved. Specifically, just two single annual meetings of all scientist and Ph.D. students, respectively, clearly do not suffice for a full exploitation of the synergistic potential of the UMR 8587. In this respect, it might also be useful to implement some instruments for monitoring and controlling in the future within the subgroups and for the UMR as a whole, in order to motivate a few less productive researchers towards new success by initiating new cooperation between the teams and launching new scientific targets. Further, more attention might be paid to the training of the technical personal and particularly the instruction of the younger scientists in affairs of intellectual property. Finally, due to its future size the collaboration between the teams of LAMBE may also profit from the *Conseil de laboratoire*.





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

### Team 1. Structure-reactivite de biomolecules: Complexes organometalliques et macromoleculaire

Team 1 has a long-standing and very profound expertise in mass spectrometry and the team is internationally recognized. In the report period, 62 papers in peer-reviewed journals have been published (1.6 publications/person-year): two in high impact journals (IF > 8) and most of the others in highly recognized journals of general chemistry or more specialized journals with good to excellent reputation in their field. Notable in comparison to Teams 2 and 3 is the significantly higher average impact factor of these papers. The performance of Team 1 is based on the human resources and the excellent experimental equipment which recently has been upgraded by an *Orbitrap* mass spectrometer. The anticipated acquisition of an ion-mobility mass spectrometer would continue this orientation and receives full support by the committee. The smooth re-orientation of Team 1 towards more biologically relevant questions is very much appreciated by the committee and also found its reflection in the scientific community. Further, Team 1 is characterized by a very large degree of cooperation, both within the teams of the UMR and with external partners. In this respect, the granted access to European Multi-user facility CLIO is a particular highlight.

With respect to the individual project proposals, all of them are sound and rated very positively; particularly the collaborative aspects within the UMR and with other groups are very strong. In fact, Team 1 may be seen as a clamp of the entire unit and this role is very much appreciated and strongly encouraged by the committee.

The first project concerning the "-omics" is at the forefront of science and the team is well-prepared to attack this challenge. However, Team 1 entered this attractive, but also highly competitive area only relatively recently, such that the international standing will only be possible to evaluate after some years of experience. The project about the use of ion/molecule reactions for the characterization of biomolecules is strong and innovative on the one hand and relies on the profound expertise of Team 1 on the other. The same holds true for the IRMPD studies (in which Team 1 belongs to the top in France and is well-recognized worldwide) and the planned ion/ion reactions, which nicely complement the tools suggested for the analysis of biomolecules.

The second set of projects about macromolecular complexes is also very strong and clearly structured. Particularly attractive are the strong collaborations with external partners on some protein complexes (MAPKs, spastine, TRIO) and the incorporation of experiments at the European Multi-user facility SOLEIL. Again, Team 1 is by and large entering a new area of research, also in a competitive field, so that the future venues need to be proven by performance. Given the profound expertise of Team 1, the committee rates these prospects very good.

The third project deals with the development of new hyphenated techniques. Here, the team can rely on its proven experience in SPR/MS and CE/MS coupling, of which the latter is rather difficult to realize and Team 1 is among the few groups worldwide having significant success in this respect. The anticipated implementation of the ion-mobility technique is perfectly appropriate for the envisioned studies of biomolecules and would offer a highly complementary tool for obtaining structural information; moreover, the ion-mobility studies offer a direct cooperation with Team 2. Furthermore, installation of an ion-mobility mass spectrometer would further strengthen the instrumental excellence of Team 1. Potential prospects can only be evaluated in the future, however, because the - strongly supported - acquisition of an IM-MS first needs to be realized.

The final project is a direct and very promising cooperation with the new Team 4 at the forefront of science. While it apparently is a high risk to attempt the detection of complexes of biomolecules at a single-molecule level, the idea is excellent, the cooperation with Team 4 gives a strong momentum and hope towards realization, and the potential perspectives are thus very high.



In summary, the entire performance of Team 1, the proposed research projects, the strong collaborations within the UMR and outside are rated very positively; in this context it is noted, however, that the performance in the "new" areas Team 1 will tackle in the future cannot be assessed at this stage. The only question which remained to the committee concerned the high workload imposed by the large number of challenging projects and collaborations on the members of Team 1, but upon directly addressing this aspect, the future team leader made clear that Team 1 will be able to master all challenges.

Recommendations for possible improvements specific to Team 1 concern the limited number of habilitated permanent researchers in the team (only 2 of the 10 permanents). Given that some of the non HDR permanents have been at Evry for up to 10 years, this is an indication that not enough is being done to incite permanent employees to pursue the HDR degree at the normal time, roughly 5 years after the Ph.D. defense. Perhaps even directly related with this is the only moderate number of Ph.D. students during the report period and like the UMR as a whole, Team 1 is strongly encouraged to increase the efforts to render the unit more attractive for Ph.D. students.

Nom de l'équipe : Structure-reactivite de biomolecules: Complexes organometalliques et macromoleculaire

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	A	A

## Team 2. Interactions des assemblages moleculaire complexes: Theorie et modelisation

Preamble. Roughly a decade ago (at about the time when the UMR changed its name to the LAMBE), the laboratory recruited a very dynamic theoretical physicist with expertise in modeling liquids and solvation who built the sizable theory group that we know today.

In the report period, the theory group was composed of 9 permanent researchers (7 UEVE/1 CNRS/1 CEA), with a very even balance between physicists and chemists. Perhaps because of its historical origins, group was built around Car-Parinello-DFT and classical molecular dynamics, coarse-grained (mesoscopic) models, and the classical density-functional theory of liquids. This gives the group the potential to do multiscale modeling from a few up to  $10^6$  atoms in a timescale from several fs to seconds. The intra group collaboration concerning the CEA is exemplary.

Part of Team 2 is very active, while some members of the team appear to be somewhat less productive. Certainly a strong point of the Team 2 are the collaborations with all three other teams in LAMBE. Team 2 has also entered actively into both French (ACI, GdR, ToxNuc) and European (COST) programs. Two *ANR Blanche* (DFTsolv and Probio) were funded during this period. Also during this period, the group produced 52 publications or a total of 1.4 publications/person-year (with some CNRS, CEA, and UEVE personnel publishing as much as on order of 4 publications/person-year and a few teaching-researchers who will hopefully publish more in the future). Two computer programs have been developed (MDVRY and Molsimu).

Three PhD theses were defended, but some lack associated publications. Being well aware of the fact that code development is slow and that fewer publications may be expected, the committee has made an effort to ascertain the reasons behind the apparent lack of submission of or tardiness in submitting articles and is not entirely satisfied with the reasons given. It should be emphasized that, when possible, students should be encouraged earlier rather than later to participate in the preparation and submission of articles associated with their theses.



Another strong point of the group is the responsibility taken in the various education programs (Licence and Master). We especially note the responsibilities for the *Physique, Chimie et Applications au Vivant* Masters program and active participation in the *European Theoretical Chemistry* Master program. In these days of declining numbers of students interested in theoretical chemistry combined with the continued need of experimental chemists for theoretical expertise, the French and European Labeled programs require our full support and Evry is doing its part well.

The committee notes that only 3 of the 9 permanents are habilitated to direct Ph.D. theses. Given that some of the non HDR permanents have been at Evry for up to 10 years, this is an indication that not enough is being done to incite permanent employees to pursue the HDR degree at the normal time, roughly 5 years after the Ph.D. defense.

The LAMBE is a bit different than many other laboratories in the sense that each group has two directors (or a director and a codirector) roughly corresponding to a major and a minor subgroup. An important change between the previous and the next 4 year periods of Team 2 is the departure of both previous directors. One consequence of this change is a partial re-orientation of the research program. A more important consequence is the loss of an important unifying personality and the replacement by necessarily less experienced members of the theory team. The committee strongly encourages intragroup collaborations on suitable projects and regular meetings. The overall impression is that the theory group has two subgroups which correspond to the division between the theoretical chemists doing DFT and classical MD and the physicists developing a coarse graining model for doing MD on large biological systems. The committee considers that fully successful multiscale modeling seems unlikely, unless the coarse grained modeling benefits to the fullest extent from DFT-MD data, and for especially biochemical problems a self-consistent update of parameters may be necessary.

The proposed projects are interesting and seem generally concrete and realistic. Most concern the application of established techniques to problems of local interest (CPMD for IR-MPD, Ehrenfest dynamics for Coulomb explosions). Some also concern newer techniques and using them for novel applications (metadynamics for describing "rare" events in the mass spectrometry of peptides and nucleides). They are interesting in context of collaborations between the teams and have resulted in funded projects (COST, GdR) of Teams 1 and 2. The continued development of the Molsimu code for localizing vibrational modes obtained from MD simulations also seems worthwhile. The committee encourages the team to reconsider the neighborhood of their MD study of the electrospray process in light of recent publications such as *J. Phys. Chem. A* 2008, 112, 9628. The ability to correctly model the *very long* scales needed to describe the collisional excitation, intramolecular energy redistribution, and final bond-breaking processes in biomolecules also seems doubtful to the auditing committee, even using metadynamics, but perhaps a multiscale approach including coarse grained dynamics can provide useful information. The proposed new project about ultrafast radiobiology will certainly profit from deeper implementation in the team including re-consideration of the applicability of the mostly physical concepts to the challenges emerging from biochemical problems. In this respect, a possible linkage might emerge from the ion/ion-reactions to be studied in Team 1.

Perhaps the most exciting but also the most high-risk proposals make use of the coarse graining approach, which is almost unique worldwide (see: *J. Struct. Biol.* 2007, 157, 579). On paper the approach is certainly innovative as also demonstrated by a *ANR jeune chercheur* grant awarded to the topic. However, too little has been published to date to judge the chances of success. The audit committee recommends more frequent publications, especially now that the technique is finally reasonably operational. We note that one of the most exciting applications (tubuline aggregation) is in-house, albeit not within LAMBE.

In summary, we feel that the theory group, now mostly composed of younger less experienced researchers, has a very great potential which is reflected by the large productivity and international recognition of a few of its members, but that the projects (or at least their presentation) deserve to be more deeply thought out, and that a serious effort needs to be made to create a sense of unity which could allow the group to move forward by taking full advantage of its diverse but complementary expertise. The committee believes, however, that Team 2 is aware of its problems and of its potential and is already beginning to take measures to resolve the remaining problems in the foreseeable future.



Nom de l'équipe : Interactions des assemblages moléculaire complexes: Théorie et modélisation

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

### Team 3. Réactivité aux interfaces dans l'environnement

The principal subject of this group is the reactivity at interfaces in the environment. The focus is on questions related to the disposal of nuclear waste, but questions of waste recycling and problems of depollution are treated as well. In the last 4 years, the team has published a large number of papers in the areas of electrochemistry, inorganic and nuclear chemistry, geochemistry and radiochemistry, in most cases in top-ranked journals of these disciplines. The national visibility is very good. With respect to international visibility, some drawback is that the CEA members of the Team are recognized as CEA, not as members of the UMR. It is noted that Team 3 hosts the largest number of HDR and Ph.D. theses of the UMR.

The first project deals with the fundamental understanding of the interactions at interfaces of natural minerals and synthetic materials. In the simulation of natural environments, an important orientation taken is to assure reducing boundary conditions. This allows the group to study redox-sensitive mineral surfaces such as siderite or pyrite. Much less clear is how the group assures the transposition of laboratory observations to expected behavior under natural conditions characterized by the simultaneous presence of multiple minerals and organic matter. Considering the profile of the UMR, a stronger consideration of natural organic matter is recommended. The committee strongly supports the strategy of going from microscopic observations (EXAFS, X-ray reflectivity) to macroscopic behavior. The work performed in this area is excellent and in this regard Team 3 is one of the leaders in the field. The analysis of thin films of minerals in electrochemical cells is promising. As suggested by the team, the logical next step is a multi-scale modeling, going from molecular level models all the way to phenomenological approaches. However, there is no explanation how the molecular modeling of interfaces will be pursued (this theme is absent in Team 2). There seems to be a conflict in the research orientation of analyzing in detail the structure of surface complexes and developing multi-site ion exchange models which are insensitive to this type of information. While such models may be justified by operational applications, they will contribute little to fundamental understanding.

The second project theme deals with reactive surfaces, in particular with corroding metals and semiconductors. The group has gained worldwide recognition in the area of long-term storage and disposal of spent nuclear fuel. Recently, however, this theme seems to be reduced to certain aspects of corrosion of  $UO_2$ . The strong electrochemical background and the notoriety of the group in the area of reactive surfaces are well acknowledged. To reach their goal of studying the continuity from elementary reactions towards the macroscopic observations of the formation of corrosion layers, the committee suggests to include as well transport processes and to benefit from the large knowledge base on transport processes available at CEA. The step towards analyzing the effects of biofilms seems interesting, but very large. The experience of the group in the area of biofilms is not documented, and the suggested investigation of bio-fuel cells has large potential, but remains vague and is linked to the rest of this subproject to an only limited extent. Finally, the orientation towards the system  $Ru/RuO_2$  opens the way to study systems of relevance to reprocessing. The committee poses the question, however, whether this implies a re-orientation of the group away from "interfaces in the environment". In the context of the studies of dilute salt solutions (metal nitrates etc.), continuation of the collaboration with Team 1 might also be fruitful, although the workload on Team 1 already is large.



The last project concerns the application of functionalized surfaces for the detection of trace elements in the environment. The group has acquired a strong knowledge base in the area of functionalized metallic surfaces and first applications to the detection of uranium are in the range of  $10^{-10}$  M; also some organic molecules could successfully be quantified. This is very encouraging and the efforts in this area are indeed strongly encouraged by the committee. However, even though some competitive effects of few ions have been studied, some doubts remain whether the group is fully aware of the enormous task of qualifying this analytical technique for environmental applications, characterized by presence of a large variety of ligands, competing ions, particulate matter, and organic molecules.

Finally, a comment on the relation between the CEA and the UMR members at Evry is indicated. The strong interest of CEA to cooperate with the University d'Evry (UEVE) is at the origin of the existence of the UMR. But in contrast to many other UMR, where scientists of different organizations work at a common place, we are faced with a situation, where, with few exceptions, scientists of CEA work at Saclay, those of UEVE work at Evry. The access to research equipment at CEA (indirectly also to SOLEIL) is an important advantage for Team 3 and the entire UMR. Without questioning the advantages for both sides, the interaction appears sometimes of more symbiotic character rather than that of a real collaboration on common themes with synergistic profits. Joint meetings are rare. Even though the committee got the impression that the relations between the staff of CEA and of UEVE are very good, and several joint research projects exists, developed research strategies seem to be those of either CEA or UEVE and not of the overall team of Team 3. An example is that the strong involvement of CEA in European projects has contributed significantly to the scientific output of Team 3, but this is not reflected in the budget of the UMR.

Nom de l'équipe : Reactivite aux interfaces dans l'environnement

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	B	A	A	B

#### Team 4. Matériaux polymères aux interfaces

Team 4 is a truly multidisciplinary research group including physicists, chemists, and biologists. The publication records are very good to excellent, and the present and future research topics are at the cutting edge of science with national leadership in the field and international visibility. In particular the project on transport of molecules through nanopores and artificial ion channels is of excellent quality. As Team 4 will newly enter the UMR, it is not part of the report, but in the same period, 45 papers in peer-reviewed journals are listed with several of them in high impact journals (1.3 publications/person-year). Notable are also four patents (also in cooperation with Team 1) and a large amount of successful grant applications in the period relevant for the report, which is quite remarkable for a group of the size and orientation of Team 4. Last but not least, the team is actively involved in the popularization of sciences which is vital for the acceptance of natural sciences in the public.

The project proposals are ambitious and the first of them is at the forefront of science. This project deals with the transport of macromolecules in nanopores and artificial ion channels. The topic itself is fascinating, the presentation was very inspiring and the students and co-workers engaged in this project make a highly motivated impression. The highly innovative character of the subproject is also reflected by a considerable donation of the CNRS for "*Prise de risque Physique et Chimie du Vivant*". In addition to these excellent perspectives with regard to the observation of translocation in real time, this project involves the development of new methods and also initiates a direct cooperation with Team 1. In brief: Top science.



Two other projects deal with the production of new polymers for gene therapy and of new types of biomaterials, including the embedding of polyrotaxanes in biomatter. Both projects are well founded on the previous experience of the team and offer innovative potential for the future. Part of these projects involve also scientists from the University Cergy-Pontoise. While these projects are basic research in the area of chemical physics and polymer sciences, both have direct links to life sciences (i.e. gene therapy, cancer treatment) and thus also offer long-term prospects for future revenue.

The chemists within Team 4 are very skilled and well-experienced. They are, however, using classical tools for polymer chemistry as well as classical polymers, probably also for historical reasons. The committee acknowledges, however, that the physicists as well as the biologists in the team very much need the chemists, and thus strongly encourage the latter to use the today's state-of-the-art in the field for the control of architectures at the molecular level (ATRP, "click" chemistry",...) for the design of new architectural polymers that could be even more beneficial for the physicists and the biologists in this team. Part of these efforts would be an upgrading of the NMR equipment which presently does not represent the state-of-art. Another point for improvement is the somewhat limited representation of younger scientists at conferences and scientific lectures, which are mostly focused on the group leaders.

Nom de l'équipe :

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+	A	A

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

### UMR 8587. Laboratoire Analyse et Modelisation pour la Biologie et l'Environnement

Based on the evaluation of the individual teams, the scientific performance of the entire UMR and its perspectives of research range from good to very good. Particularly strong points are the intense collaboration of Teams 1 and 2 with the others and the potentially ground-breaking cooperation between Teams 1 and 4. The total publication records of the UMR and its international visibility might still be improvable, however.

While the management of the separate teams is very good to excellent (with a certainly only temporary exception in Team 2 due to re-structuring), the overall management of the UMR 8587 still offers room for significant improvement. Specifically, the scientific interaction of the teams should be strengthened further by more joint seminars, lectures etc., in order to fully exploit synergisms between the research units. Likewise, instruments for monitoring and controlling should be installed to further improve future performance, to identify weaknesses, and motivate the researchers towards tackling new frontiers.

As already mentioned above, the UMR has a solid base of permanent researchers for the realization of the projects and the proposed integration of the additional Team 4 is rated positively without any reservations. With respect to human resources it is desirable, however, if the management of the UMR as well as the University d'Evry could try as much as possible to increase their efforts to render the lab more attractive for Ph.D. students. The same holds true for the number of habilitated scientists in the teams, though this point is less important. The third concern with respect to the human resources concerns the efforts of both the UMR and the Université d'Evry to support excellence in the teams, which, for example, could be reflected by an application for an ERC Starting or Advanced Grant.



With respect to communication, the level and amount of inter-team meetings and scientific discussions is suggested to be improved in the future and the same holds true for the embedding of the scientists from CEA Saclay in the scientific life of the entire UMR, not just Team 3.

## 6 • Recommendations and advice

### — Strong points :

- strong interdisciplinary character of the UMR
- integration of Team 4
- almost unique cooperation between university and a state research organization (CEA)
- economically relevant targets in Team 3
- good to excellent publication and conference records in the report period (also several publications in high-impact journals)
- attractive research proposals (among these a very attractive high-risk / high-gain project between Teams 1 and 4)
- excellent equipment in Team 1
- access to European Multi-user facilities

### — Weak points :

- attractiveness for Ph.D. students
- number of HDR
- intergroup communication and meetings
- communication within Team 2
- implementation of the CEA researchers in the scientific life of the UMR
- focusing of projects in Teams 2 and 3
- engagement in "big" European projects
- training about intellectual property
- instrumentation in Team 4 (NMR)

### — Recommendations :

- render the UMR 8587 more attractive for new Ph.D. candidates
- improvement of scientific life between the teams
- support of excellence
- closer integration of CEA researchers



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	A	A	A	A





**Université d'Evry-Val-d'Essonne  
Cabinet de la Présidence**

Affaire suivie par :  
Emery Olivier  
Téléphone :  
01.69.47.80.46

Evry, le jeudi 16 avril 2009

Le Président de l'Université

à

Monsieur Jean-François DHAINAUT  
Directeur de l'AERES

*Objet : Rapport d'Evaluation du Laboratoire Analyse et Modélisation pour la Biologie et l'Environnement (LAMBE UMR 8587) S2100015506*

Monsieur le Directeur,

Vous m'avez transmis le rapport d'évaluation du laboratoire LAMBE dirigé par le Professeur Jeanine TORTAJADA.

Vous trouverez ci-joint, en réponse au rapport qui lui a été adressé, les remarques et commentaires de la Directrice de ce laboratoire.

Je m'associe aux remerciements pour la qualité de cette expertise qui reflète le sérieux du travail accompli par les experts et les représentants de l'AERES.

Je me réjouis de la teneur très positive de ce rapport et souscris à l'ensemble de l'analyse de cette unité. Je prends note des recommandations formulées concernant notamment l'attractivité des doctorants.

Sur la base des conclusions et des recommandations formulées, l'université s'efforcera d'accompagner au mieux ce laboratoire dynamique et reconnu pour son positionnement original et pluridisciplinaire.

Je vous prie d'agréer, Monsieur le Directeur, l'expression de mes salutations distinguées.

Le Président de l'université  
d'Evry-Val-d'Essonne

Richard MESSIN



L'Administrateur Général



Monsieur Pierre GLORIEUX  
Directeur de la Section des Unités

AERES  
20, rue Vivienne  
75002 Paris

Saclay le 20 avril 2009

**Objet :** Observations du CEA sur le rapport d'évaluation du Laboratoire d'Analyse et Modélisation pour la Biologie et l'Environnement, 8587  
(Référence : EVAL-0911975C-S2100015506-UR-RPRELIM)

**N/Réf. :** DPG/AN/mos/2009-123

Monsieur le Directeur,

Je remercie tout d'abord l'AERES pour la qualité du rapport d'évaluation et pour la pertinence des recommandations qui ont été faites.

Vous trouverez, ci-joint, les commentaires faits par Madame Jeanine Tortajada, directrice du Laboratoire Analyse et Modélisation pour la Biologie et l'Environnement (UMR 8587), sur ce rapport d'évaluation.

En tant qu'Administrateur Général de l'Etablissement CEA, ce rapport n'appelle pas de commentaires particuliers de ma part. Je prêterai la plus grande attention à la mise en œuvre des actions qui permettront de répondre aux recommandations formulées par l'Agence.

Je vous prie d'agréer, Monsieur le Directeur, l'expression de mes meilleures salutations.

A handwritten signature in black ink, appearing to read 'Bernard Bigot'. The signature is written over a horizontal line that extends to the right.

Bernard BIGOT



Laboratoire Analyse et Modélisation  
pour la Biologie et l'Environnement



UMR 8587

*Jeanine Tortajada, Directrice*

## ANSWER AND COMMENTS ON THE AERES EVALUATION REPORT OF THE LAMBE (UMR 8587)

The members of the unit thank the Evaluation Committee for its thorough and constructive report. We thank the committee for the overall positive appreciations and we appreciate the frank comments and remarks in relation to the scientific projects, the organisation and the management of the unit. We agree with most of the comments, conclusions and constructive recommendations and we will make the best use of them, to pursue the ongoing evolution of the LAMBE during the next years. We will endeavour to render the UMR more attractive banking on our multidisciplinary research recognised by the committee as “almost unique in France”. In spite of the hard competitiveness of the scientific environment, we will work for increasing the number of Ph.D students with the assistance of our Supervisors (University and CEA). We plan also to develop much more interactions between the four teams by increasing collaborative synergies.

We are also pleased that the Committee underlines as strong point, the integration of team 4. This team which develops topics at the cutting edge of science brings a more multidisciplinary dimension, reinforced by the integration of three biologists of the University of Cergy-Pontoise.

Although we appreciate the overall analyses on teams' activities we wish to address specific comments, concerning some questionings and remarks.

♦ As underlined by the committee, Team 1 will focus its efforts to significantly increase the number of HDR permanents. 3 new HDR defences are already planned for 2009. Team 1 thanks the committee for appreciating its global vision and effort for promoting a lively network within the teams of the UMR and outside, as well as for an integrated multidisciplinary approach of chemical processes in a biological context.

♦ The committee has pointed that Team 2 has developed and improved methods based on molecular dynamics simulations that ultimately lead to a wide range of time- and length-scale representations (TD-DFT dynamics, Car-Parrinello dynamics, classical dynamics, solvation models, coarse-grain dynamics) on pertinent and diversified subjects (radio-biology, vibrational spectroscopy, reactive collisions, electrospray evaporation, protein recognition, proteins organisation). That is almost unique in French laboratories. We thank the committee for its encouragements regarding these-performed researches. We also thank the committee for the recognition of the collaboration with the CEA, which will be even reinforced in the near future.

We feel nonetheless that some clarifications have to be done on certain scientific points arose by the committee.

- On our new ongoing work on *electrospray ESI* the committee suggests that we use atomistic based simulations. We have chosen the mesoscopic general approach because our objective is to give a general comprehension of the ESI. This is in line with J. Jortner's philosophy who has already applied this approach to the Coulomb explosion of simple charged droplets (Mol. Phys. 104:1227, 2006). We are aware that this approach may appear risky, but this path has to be explored.

- For the *CID reactive collisions*, we do not propose anything related to metadynamics, that is used by us in a completely different context, thus maybe the confusion from the committee. We disagree with the committee's suggestion concerning a coarse-grain approach for the long time-scale coupling, because chemical reactions (proton transfers and covalent bond breakings) and isomerisations still take place at such long time-scales. This has to be properly modeled.

- On our *radiobiology investigations*, the committee suggests that we should combine this subject with ion/ion reactions performed by Team 1. These experiments unfortunately do not deal with comparable energetics, and for that purpose we already collaborate with experimentalists of these high energy collisions.

◆ Several projects have been proposed by Team 3 dealing with reactivity at interfaces in the environment and we want to answer to few comments and questioning of the Committee.

- The molecular-scale characterizations of interfacial atomic structure are currently performed by UMR team members in collaboration with other CEA groups to explore the potential of ab initio modelling of interfaces. We plan to carry on these studies by using theoretical approaches developed by members of team 2.

- Concerning the theme dealing with reactive surfaces, the group has not an extended experience in biofilms, as pointed out by the committee; it is in fact a future development proposed by the group, in accordance with its background. It is with this objective that the group welcomes a new member, D. Féron, who has an extended experience in the biofilms area (he is member of the editorial committee of the journal Biofouling), in the biocorrosion domain (he has edited a special issue of *Electrochimica Acta* – Vol 54, issue 1, December 2008- on biocorrosion of metallic materials) and in the application of biofilms for biofuel cells (several patents). The investigations on biofuel cells will be focused on the reactivity of the interfaces with biofilms and more precisely on the new concept of electro-active biofilms (EA-Biofilms).”

- The strong electrochemical background of the UMR will be also developed on the behaviour of ruthenium, not only in a nitric concentrated media, but also after its immobilization in a dedicated metallic waste form (long-term behaviour under geological disposal conditions).

- The background in environmental, analytical and actinide chemistry of the UMR'scientists will be the basement to develop functionalized surfaces with new CEA members which joint the UMR (C. Beaucaire, J. Ly, Y. Lazack and D. Doizi).The aim is to detect toxic and trace elements in the environment, through direct or indirect derivate circuits including specific ligands and separative-molecules.

◆ Concerning the polymer chemistry strategy of Team 4, most of the envisioned polymers are thought on a "structure-biological activity" relationship, which means that the investigated polymerization chemistry mainly focuses on ring opening polymerization. The click chemistry tool is currently used in our lab for the design of new ligand molecules, and controlled radical polymerization is carried out in collaboration with an australian team. Indeed, some elegant polymer architecture are just being published in advanced material, recognized as a high impact journal (IF>8).

We want to add that the actual NMR spectrometer corresponds to our current needs, knowing that our team has access in the same building, to a 600MHz apparatus when needed.

Evry, the 10<sup>th</sup> April 2009



Jeanine TORTAJADA