Chimie de la matière complexe

Rapport Hcéres

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

Research Units Department

AERES report on
Unit:

Chimie de la Matière Complexe

Unit Acronym CMC

Under the supervision of the following institutions and research bodies:

University of Strasbourg

CNRS

January 2012

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

Section des Unités de recherche

Le Président de l'AERES

Didier Houssin

Section des Unités de recherche

Le Directeur

Pierre Glaudes

Unit

Name of unit:	Chimie de la Matière Complexe
Acronym of unit:	CMC
Label requested:	UMR
Present no.:	UMR 7140
Name of Director (2009-2012):	Mr Mir Wais HOSSEINI
Name of project leader (2013-2017):	Mr Mir Wais HOSSEINI

Members of the committee of experts

Chair:	Mr Ludovic JULLIEN, Paris
Experts:	Ms Ulrike ALEXIEV, Berlin, Germany
	Mr Serge ANTONCZAK, Nice
	Mr Marco DATURI (representative of CoNRS)
	Mr Dominique MASSIOT, Orléans
	Mr Luc MORIN-ALLORY, Orléans
	Mr Rinaldo POLI, Toulouse
	Mr Claude PIGUET, Genève, Switzerland
	Ms Anna PROUST (representative of CNU)
	Mr Rolf SAALFRANK, Erlangen, Germany
	Ms Jeanine TORTAJADA, Evry

Representatives present during the visit

Scientific Delegate representing AERES:

Ms Gilberte CHAMBAUD

Representative(s) of the unit's supervising institutions and bodies:

Mr Daniel GUILLON, UDS

Mr Claude POUCHAN, INC-CNRS

Report

1 • Introduction

Date and conduct of visit: 12-13th January, 2012

The visit took place over two days, the 12th and 13th January 2012. It started with a general presentation of the previous research unit by its director. Then each group of the future research unit presented its past achievements as well as its project for the next contract 2013-2017. The reasoning leading to the new perimeter of the unit as well as the forthcoming organization of the common facilities (Federation) were subsequently exposed by their respective directors. These speeches were followed by a general discussion with all the staff of the laboratory. The remaining of the first day was dedicated to visits of the laboratories and discussions with the group members in front of posters. After a discussion between the institutional representatives (UDS, CNRS) and the committee members, the second day was dedicated to internal discussions to the committee.

History and geographical location of the unit, and overall description of its field and activities:

The laboratory "Chemistry of complex matter" ("Chimie de la matière complexe") is a 'Unité Mixte de Recherche' CNRS / Université de Strasbourg (UMR 7140). It results from the incorporation of three new teams originating from the UMR 7177, to the former UMR 7140 "Molecular tectonics of solids" ("Tectonique Moléculaire des Solides"). The laboratory aims at addressing complexity of chemical matter envisaged as the next relevant organization level in chemistry after molecules and supramolecules. The activity of the laboratory will cover theory, syntheses, analyses, and physicochemical investigations.

Management team:

Director: Mr Mir Wais HOSSEINI

Adjunct-Directors: Mr Jean-Marc PLANEIX together with Ms Petra HELLWIG in the future unit.

Unit workforce:

Workforce	Number on 06/30/2011	Number on 01/01/2013	2013-2017 Number of producers**
N1: Professors or assistant professors	13	13	13
N2: EPST or EPIC researchers	6	6	6
N3: Other professors and researchers	0		
N4: Engineers, technicians and administrative staff *****on a permanent position	4		
N5: Engineers, technicians and administrative staff ***** on a non-permanent position	0		
N6: Postdoctoral students having spent at least 12 months in the unit	14		
N7: Doctoral students	24		
N8: PhD defended	23		
N9: Number of Habilitations to Direct Research (HDR) defended	2		
N10: People habilitated to direct research or similar	12	12	
TOTAL N1 to N7	**61**	**19**	**19**

* **If** different, indicate corresponding FTEs in brackets.

** Number of producers in the 2008-2011 period who will be present in 2013-2017.

2 • Assessment of the unit

Overall opinion on the unit:

The research unit unifies five complementary teams around the common and promising topic of Chemistry of Complex Matter, which will be practiced along various nationally and internationally-recognized approaches. Although they will be totally independent with respect of the use of their financial resources and their scientific interests, the team members share a common dynamic spirit and the enlarged perimeter of the new UMR could provide interesting opportunities for all its five components. The unit should eventually benefit from the dynamics and the supports from the Labex"Chemistry of Complex Systems" and from the Idex allocated to Strasbourg University. All these elements have convinced the committee of experts of the relevance of the unit contour.

Despite such favorable features, the committee members have been also concerned by several weakening elements. The five constitutive unit teams are presently dispersed geographically, which does not facilitate the emergence of a common culture. Several unit members cumulate local and national responsabilities much beyond the relative significance of the unit size. Although this result probably expresses their concerns for community interests, this engagement is at the same time a risk for securing the future of the unit by addressing the most ambitious and time-demanding scientific projects. The committee members eventually noted that currently non existing or partial technical and instrumental support will need to be implemented to fulfill all the unit projects.

Strengths and opportunities:

Timely relevance of the topic of Chemistry of complex systems.

Expertise and complementarity of the five research groups.

Quality of the scientific production.

Quality of human resources.

The five teams share a common dynamical spirit for organizing and practicing science as well as a consensus about governance principles.

Participation to the Strasbourg University Idex and to the Labex "Chemistry of Complex Systems".

Weaknesses and risks:

No continuity of the unit premises.

Extremely important involvement in training and structuring activities at the regional and at the national level.

Lack of technical support in two groups.

Lack of defined strategy for facilitated access to platform mass spectrometers

Recommendations:

Although approving the pragmatic and science quality-driven approach of the unit, the committee members strongly encourage all the unit members to aim at synergism. In particular, this support could materialize in addressing a few meaningful high-level scientific challenges, which would be also valuable to create a unit spirit. The unit global investment in local and national policies should also be more equally shared among the unit members to reorient more time and energy to the emergence and the developments of new projects.

3 • Detailed assessments

Assessment of scientific quality and production:

The research unit unifies five teams around a common scientific motto (Chemistry of Complex Matter). Although more restricted than in the context of the Labex "Chemistry of Complex Systems" to which two unit teams participate, the unit interpretation of complexity is relevant and in phase with several recent developments in chemistry.

The gathered multidisciplinary and complementary expertises (organic/inorganic/biological chemistry, material science - crystal engineering, analytical and physical chemistry – bioelectrochemistry, X-ray diffraction, IR-, MS spectroscopy, and theory – chemoinformatics, PACHA) are recognized in their respective fields, both at the national and international levels.

The enlarged perimeter of the new UMR could provide interesting opportunities for all its five components. They have been convincingly evoked by the unit director as well as by the team leaders during the visit. Although approving the pragmatic and science quality-driven approach of the unit director, the committee members strongly encourage all the unit members to aim at synergism. In particular, this support could materialize in addressing a few meaningful high-level scientific challenges.

The quality (documented by numerous publications in previewed international journals with good to high impact factors) and the quantity of publications, communications, and dissertations are globally very good. All the members of the research unit are authors of documents.

Assessment of the unit's integration into its environment:

The five unit teams have mainly motivated their research by progress at the cutting edge of fundamental knowledge. Transfer of knowledge to the industrial sector has not been put forward as a major motivation of scientific projects. However, one should note that two groups have already very good contacts with major industrial partners. This perspective should be encouraged and extended to other teams to diversify funding resources and enlarge professional employment perspectives for the students and post-docs trained within the unit.

In contrast, several members of the unit are strongly engaged in various and highly significant organizational activities relying on their expertise and dynamism (chairing the Collegium, adjunct director of the Strasbourg Foundation and "Chemistry of Complex Systems" Labex, direction of the Chemistry UFR…).

The five teams globally do not suffer from any major lack of financial support. In particular, they benefited from significant local grants during the last contract, which mainly originated from the Strasbourg Foundation of Chemistry. The recent Strasbourg success to the Idex selection is prone to sustain this trend. Two groups additionnally belong to the recently supported Labex "Chemistry of Complex Systems", which should also contribute to secure the financial support of their scientific activity in the forthcoming years. Despite such opportunities, the committee members strongly encourage the unit teams to apply to external financing sources (in particular national – ANR – and european – ERC, Marie Curie, etc.).

Assessment of the research unit's reputation and drawing power:

The research unit's reputation and attractivity is well documented in a list of prizes and distinguished awards, invitations to international and national events and also by the listed invited professors, postdocs and high-level students of national and international origin.

There exist various collaborations of excellence with national and international laboratories (Frankfurt, Illinois, Pennstate, San Francisco, ANKA Karlsruhe, BESSY Berlin, Freiburg, etc). The unit is also engaged in an active policy of institutional partnership.

Assessment of the unit's governance and life:

The new unit results from the association of the two original teams from the UMR 7140 with three new teams originating from the UMR 7177. Despite this major change, the committee has been convinced that the five teams share a common spirit and organizational rules about science practice so as to build a coherent laboratory.

The unit management relies on the director, two adjunct-directors, a board of principal investigators and the unit council (including all the permanent members + 2 representatives elected among non-permanent members). The task force has been efficient to conceive the unit project, which was discussed within each team. Further effort should be now directed to favor interactions between the permanent members, both to share the unit project and to support the emergence of common scientific projects. From the latter point of view, the unit presently suffers from the lack of premise continuity, which should be remediated in the course of the next contract. In relation to the present geographical dispersion, the committee members have estimated that the unit should benefit from the organization of a real "Conseil de laboratoire" obeying the CNRS rules.

The five research groups will be scientifically independent entities. Further scientific activity and emergence of new common projects will be mainly stimulated by organizing three one-day symposia per year during which the team members will present their results and achievements. Although recognizing the relevance of the pragmatic attitude of the unit director, who will make strong efforts to support excellent emerging projects, the committee recommends the additional organization of prospective seminars devoted to identifying research opportunities within the unit.

The unit members are strongly involved both in educational activities and structuring of regional and national research. Whereas this involvment is to be generally encouraged, the committee members have estimated that it was probably excessive with regards to both the size of the unit and the existence of other human resources on the esplanade site of Strasbourg University.

Assessment of the strategy and 5-year project:

The five constitutive teams have defined a common referential for practicing and supporting scientific activity. This referential has been materialized under the timely motto of complex matter organizations, which covers various interpretations within the unit. In fact, the five research groups will be scientifically and financially independent entities. Recurrent financial supports and fellowships originating from the university or the CNRS will be shared on the basis of the number of permanent staff members.

Assessment of the unit's involvement in training:

The unit members are strongly involved in training at all stages of the university curriculum. They are specifically in charge of numerous pivotal management responsibilities at the Bachelor, Master, and Doctoral School levels.

4 • Team-by-team analysis

Team 1: Tectonique Moléculaire

Team leader: Mr Mir Wais HOSSEINI

Workforce

Workforce	Number on 06/30/2011	Number on 01/01/2013	2013-2017 Number of producers**
N1: Professors or assistant professors	5	5	5
N2: EPST or EPIC researchers	2	2	2
N3: Other professors and researchers	0	0	0
N4: Engineers, technicians and administrative staff * on a permanent position	3.7	4	
N5: Engineers, technicians and administrative staff * on a non-permanent position	0		
N6: Postdoctoral students having spent at least 12 months in the unit	5		
N7: Doctoral students	7		
N8: PhD defended	13		
N9: Number of Habilitations to Direct Research (HDR) defended	1		
N10: People habilitated to direct research or similar	7	7	
TOTAL N1 to N7	**22.7**	**11**	**7**

* **If** different, indicate corresponding FTEs in brackets.

** Number of producers in the 2008-2011 period who will be present in 2013-2017.

• Detailed assessments

Assessment of scientific quality and production:

The research activity of the Molecular Tectonics group is of considerable quality and original. It has been until now and continues to be of purely fundamental nature (basic curiosity-driven research). It deals with a bottom-up approach to the synthesis of functional molecular materials based on the control of intermolecular associations and self-assembly processes driven by recognition. This approach allows to iteratively assembling various tectons to yield crystalline products (1D-, 2D-, 3D-coordination networks, porous crystals by formation of cavities and channels through H- or coordination bonds). Also crystals of crystals accessible through 3D epitaxial growth were investigated. New developments include surface patterning (collaboration with ISIS, Strasbourg) and the design of luminescent liquid crystals (collaboration with IPCMS, Strasbourg). In addition, two new fields of research have been initiated: the first one deals with molecular motion and the conception of molecular gates and turnstile processes based on functionalized porphyrins. The second deals with molecular photonics systems emitting in the NIR, based on the complexation of lanthanide cations by porphyrin bearing chelating units.

Some guiding principles in terms of potential applications exist (see projects below). Citation of the team publications by other groups is moderate (average of 6.97 citations per published article in 2007-2011; 30 % of these are self-citations; due to the small size of the international community in this area), showing a good but not exceptional impact of the research.

The team has published 62 articles in international refereed journals of high average impact factor (4.56 based on the journal IF of 2010) for the period 2007-2011. For a group of 7 "publishing permanent members", this translates into 1.77 publications per permanent member per year. 13 theses have been defended in the 2007-2011 period. Considering that a large fraction of these publications are communications, the productivity of the team can be considered as quantitatively moderate, although qualitatively excellent. The scientific quality of the contributions has been recognized in the participation in the Labex Chemistry of Complex Systems, which will be directed by M. W. Hosseini. All permanent researchers and research faculty are "publishing". It is worth to note the strong contribution of Research Engineers.

- ### Assessment of the research team's integration into its environment:

The research carried out by this team is of purely fundamental nature. No industrial partnership or socioeconomic relation has been sought. Most of the researchers of Teams 1 and 2 are involved in the dissemination of scientific knowledge in schools or to the general public, for example as regional coordinator of the 2011 International year of Chemistry.

The unit (UMR) has been successful in attracting financial support from institutional and local sources (UdS, CNRS and especially RTRA-CPER) but not so much from external sources. The scientific report of the team and self-evaluation of the UMR are poorly organized, because external funding from ANR (projects FERROMOL and PMOEAH) and international (project FUMASSEC) sources are shown in Table 3.1 (AERES financial resources table) but nowhere else in the document these contracts are mentioned. In summary, small participation in 2 ANR projects but no project held by the group.

The group, on the other hand, is extremely well integrated into its local environment at the teaching and administrative levels, with some members having served or still serving the University on important roles (Doctoral School, Collegium, RTRA-icFRC, UFR, Scientific Council, …) and thus providing an essential contribution to the organisation and development of chemistry at the University of Strasbourg.

- ### Assessment of the research team's reputation and drawing power:

The group leader enjoys a very strong international profile. He has received a Prize from (and has been elected honorary member of) the Romanian Chemical Society, and a binational (franco-italian) prize of the Italian Chemical Society. He acted as editor and as member of the editorial board of Chem. Commun. 2000-08; he is co-editor in chief of New J. Chem., and since 2010 member of the advisory board of Crystal Engineering and member of the editorial board of Crystal Engineering Communications. He also had numerous invitations to deliver lectures at international conferences and in other research institutions (48 and 52, respectively) both in France and abroad. He is an elected member of CNU (section 32). At the national level, he has received the silver medal of CNRS in 2011 and is a senior member of IUF since 2004. A younger Professor in the group has also been recognized by the election as junior IUF member. Almost all of the research leaders have given invited talks in international congresses. One other team member participates to the CNRS National committee (section 14). Several group members are heavily involved in pedagogical and organizational tasks. A total of 8 symposia have been organized during the period.

With these premises, the group has an attractive profile. It has hosted 5 post-doctoral fellows (3 from abroad), 10 defended PhD (5 from abroad) and trained 7 PhD students (3 from abroad) in the reference period 2008-2011.

The group entertains a few collaborations with French and foreign institutions (New York University, Marie Curie Training Program), but none of these appears to be part of a structured (funded) programme. The majority of the scientific production is proper to the team.

- Assessment of the strategy and 5-year project:

The project part is the best part of the report concerning this team. It is imaginative, broad in scope, and opening to a multitude of potential applications. Even though most of the proposed research remains of purely fundamental nature, specific applications are taken as guide to orient much of it (separation of enantiomers of gaseous inhalation anaesthetics, asymmetric catalysis, luminescent properties,...).

The synthetic strategy for the iterative construction of complex matter from various tectons is based on self-complementary building blocks (complex as ligand and complex as metal strategy introduced by Balzani) or complementary couples containing in their backbone recognition sites and a construction algorithm. Relying on the expertise gathered in the tailor made construction of complex periodical architectures, the presented project aims at bridging the gap between structural and functional networks. The first two projects (P1 and P2) thus put forward the valorization of previous results obtained on porous networks and the possibility to design chiral cavities. The first one is based on the ability of $ZnSiF_6$ to form inorganic pillars to be connected by four flexible enantiomerically pure helical organic tectons and to be tested in chiral separation of anaesthetics enantiomers. The second one proposes decoration by chiral substituents of the hexagonal channels obtained through the assembly of functionalized porphyrins, for the separation of chiral alcohols and enantioselective transformations. Efforts directed towards the elaboration of heterometallic multifunctional networks (porous and luminescent, P3 project) will be pursued, while surface patterning (directional 1D or 2D) will be tackled through the organization of porphyrins bearing mono and tri-dentate coordination sites (P5 project). Porphyrins, which constitute the stator backbone of molecular turnstiles developed in this group, will be further poly-derivatized and investigated for pH triggered directional movement in the P6 project. Furthermore, the P4 project will make use of new protonated cationic tectons based on bisimidazolium, potentially fluorescent and photoisomerizable, for the elaboration of crystals of crystals and reticulation of (bio)polymers bearing carboxylate or sulfonate groups.

The projects will certainly benefit from the skills of the various research groups brought together in the new research structure. Some of them are sketched: understanding of energetics in the solid state following a previous collaboration with already published results; monitoring of the early stage of crystal formation by mass spectrometry, which is an emerging and challenging topics in cluster chemistry; constitution of a data base of tectons and of already characterized molecular architectures to be exploited for the design of new relevant combinations ; tackling of molecular motion directionality taking advantage of the expertise in 2D IR techniques, although this idea is not really detailed.

Conclusion:

The research group will be embedded in a research unit composed of five teams focused on a common scientific topic “Chemistry of Complex Matter”. Although all the team members will be totally independent with respect of the use of their financial resources and their scientific interests, the Committee strongly encourages all the unit members to aim at synergism. The research proposal convincingly demonstrates that the recognition of similarities in the synthesis of complex matter allows prediction of potential results in related cases. It is clear that this approach sometimes will lead to serendipitous results, which after elucidation provide new insights useful for advanced studies.

All the projects proposed are very challenging and of high scientific quality with significant potential for possible future applications. This is especially true for P1 “Chiral separation of racemic anaesthetics by porous crystals with homochiral space”. Especially for this issue the presentation of preliminary results would have been relevant.

Finally, the highly interdisciplinary character of the research of the group and the concentrated use and interplay of the broad spectrum of spectroscopic facilities and expertise (inorganic/organic chemistry, material science, crystal engineering, bioelectrochemistry, X-ray diffraction, IR-, MS spectroscopy, theory) of the unit besides the successful development of the “Chemistry of Complex Matter” on the basis of tectons, guarantee an excellent broad training for young chemists and present a nice example of fundamental ”curiosity-driven research”.

Team 2: Chimie Moléculaire du Solide

Team leader: Mr Marc HENRY

Workforce

Workforce	Number on 06/30/2011	Number on 01/01/2013	2013-2017 Number of producers**
N1: Professors or assistant professors	3	3	3
N2: EPST or EPIC researchers	0		
N3: Other professors and researchers	0		
N4: Engineers, technicians and administrative staff * on a permanent position	0.2	0,2	
N5: Engineers, technicians and administrative staff * on a non-permanent position	0		
N6: Postdoctoral students having spent at least 12 months in the unit	0		
N7: Doctoral students	0		
N8: PhD defended	3		
N9: Number of Habilitations to Direct Research (HDR) defended	0		
N10: People habilitated to direct research or similar	1		
TOTAL N1 to N7	**3.2**	**3.2**	**3**

* If different, indicate corresponding FTEs in brackets.

** Number of producers in the 2008-2011 period who will be present in 2013-2017.

Detailed assessments

- Assessment of scientific quality and production:

The team consists in three permanent members [1 professor and 2 assistant professors - MDC] with three PhD students and no post-doctoral fellows over the 2007-2011 period. The activity of the team is mostly recognized for the long-term development of the PACHA software package (since 1993) that allows assessment of the thermodynamic stability of self-assembled solids. The strength of this approach is its ability to consider extended systems for which the application of DFT based approaches still remain difficult or impossible. This is especially the case of supramolecular assemblies involving heavy metals and/or numerous water molecules with applications to the Ti based alkoxides, aryloxides or polyoxometalates including giant POMs like the $[Mo_{132}O_{372}(CH_3COO)_{30}(H_2O)_{72}]^{42-}$ (Mo_{132}) nanocapsule. The organization of the water molecules and their dynamics inside the capsule was studied by neutron diffusion techniques and spin echo NMR in collaboration with the CEA Saclay, while the mechanism of its self-assembly was tackled by DFT calculations in collaboration with the Laboratory of Quantum Chemistry in Strasbourg. These investigations have underlined the role of water during self-assembly and have proposed a path for the formation of the pentagonal units and the dimeric linkers essential to the capsule self-assembly. Although interesting, the development of the chemistry of Ti-based alkoxide and aryloxide complexes and their subsequent study by 1H DOSY NMR spectroscopy with discussion of the diffusivity in terms of the shape of the solvated objects are less original and less visible with a clear lack of identified perspective of applications.

Although of good or even very good quality [Angewandte Chemie] the scientific production of the team remained rather modest in the 2007-2008 period with a remarkable increase in 2009-2011 [11 out of 16 publications]. Most of these articles correspond to collaborations at national and international level. Only one out of the 3 PhD theses has currently given rise to a publication. This can be considered as a poor outcome that obviously could largely be improved. It should be noted that one member of the group published 7 articles considered as not being part of the UMR activity.

Concerning the PhD students, none seems to have received financial fellowship support.

- Assessment of the research team's integration into its environment:

No industrial partnership or socioeconomic relation is reported in the document and no mention is given of any ANR or contract providing financial support for the group's activity. There exists an ongoing collaboration project with EMPA for the incorporation of POMs in membranes.

One assistant professor of the group is Director of studies for L1 and involved in numerous education related charges. She supervises the elaboration of short movies for educational purposes and was a key person for the local organization of the Year of Chemistry. This activity includes a record of "grand public" conferences on water.

- Assessment of the research team's reputation and drawing power:

The group appears to have a rather limited international visibility. Only 4 invited conference talks and 7 oral presentations were given in the reference period. Only two of the invited presentations and one of the oral presentations were genuine scientific talks in an international context. The report only mentions 3 poster presentations with a single international event leading to a limited visibility of the results of the team. The group leader is member of the editorial board of Inter. J. Mol. Science since 2002 and of Water since 2008. No other particular distinction is mentioned in the report. No post-doctoral associate was recruited in the reference period. Even though the group entertains a wide and fruitful network of collaborations based on the use of the PACHA software with several well-known international groups, none of these appears to be part of a structured (funded) program.

- Assessment of the strategy and 5-year project:

The project is presented in four sub-projects, two of them appearing to be the continuation of on-going research. The main project (P4) is in-line with the already recognized expertise of the team; it consists of the up-grading of the PACHA software to include apolar molecular tectons and entropic contributions so as to address dynamic aspects of self-assembly. The adaptation of the code to existing molecular dynamics codes can possibly establish a collaboration with the team 5. The project P3 on ^{1}H DOSY NMR of POMs (M = Ti, Mo) focusses on the investigation of reliable correlations between diffusion coefficients and their molecular weights; it will likely benefit from complementary data provided by mass spectrometry (Team 4). Two other projects propose to extend the chemistry of oligophenylenes in several directions: self-assembling of 2,2' biphenol containing oligophenylenes to lead

to porous and flexible purely organic frameworks (P1); elaboration of photo-sensitive Ti(IV) porous hybrid materials based on multitopic resorcinol ligands separated by oligophenylenes (P2).

Most of the expected potential of the project is based on the recognised expertise of the PACHA software development and its possible evolutions.

Conclusion:

The project announced by this team is not fully convincing and even the realisation of part of it would require a profound change. Even with a globally good quality of publications for its permanent members, this small research team suffers from a lack of visibility exemplified by the too limited number of oral and poster presentations at the international level. The development of the proposed project has to take benefit of possible synergies with the research groups joining the new UMR structure but will certainly require financial support, at least through local or national funding.

Team 3:	Bioélectrochimie et Spectroscopie
Team leader:	Ms Petra HELLWIG

Workforce

Workforce	Number on 06/30/2011	Number on 01/01/2013	2013-2017 Number of producers**
N1: Professors or assistant professors	2	2	2
N2: EPST or EPIC researchers	0		
N3: Other professors and researchers	0		
N4: Engineers, technicians and administrative staff * on a permanent position	0		
N5: Engineers, technicians and administrative staff * on a non-permanent position	0		
N6: Postdoctoral students having spent at least 12 months in the unit	4		
N7: Doctoral students	8		
N8: PhD defended	3		
N9: Number of Habilitations to Direct Research (HDR) defended	0		
N10: People habilitated to direct research or similar	1		
TOTAL N1 to N7	**14**	**2**	**2**

* **If** different, indicate corresponding FTEs in brackets.

** Number of producers in the 2008-2011 period who will be present in 2013-2017.

Detailed assessments

- ### Assessment of scientific quality and production:

This team is constituted by one professor and one assistant professor. It investigates the role of proteins in central chemical processes of energy transduction in biological cells (field of molecular bioenergetics), via advanced spectroscopic techniques (IR, Raman), combined with electrochemistry and photochemistry tools. The topic is highly interesting and timely, addressing numerous fundamental knowledge issues and practical applications.

The team has published an important number of papers (40), corresponding to an excellent average of 4.7 papers per permanent team member and per year. The targeted journals are the main titles in the domains of biochemistry and physical-chemistry. The team leader has also participated to 5 books on electrochemistry, spectroscopy and biological processes. 4 invited conferences during the evaluation period can be considered as a good achievement, taking into account the size and the recent constitution of the team, while 29 oral communications and 28 posters represent an excellent score.

The group leader has also participated to the organisation of 5 symposia, at the international and local scale.

- ### Assessment of the research team's integration into its environment:

The team is involved in several industrial and collaborative contracts, evidencing the interest generated by its research in a broader audience than the mere academic partnership. In addition to local support, the group has been particularly successful with respect to its application to numerous calls (Chaire d'excellence ANR, FRM,…). Beyond the comfortable budget generated by its projects, the team benefits from an excellent network of collaborations in France and Germany.

- ### Assessment of the research team's reputation and drawing power:

The team leader has obtained a "chair of excellence" from ANR and is a young member of the IUF. The group has attracted an important number of researchers and students, many of them from abroad.

Several collaborations with laboratories in France and abroad seem well-established.

- ### Assessment of the strategy and 5-year project:

The main project of the team is to study enzymes at the molecular level (in particular their reaction mechanisms), upon developing new and challenging spectroscopic tools. For example, using the far IR region to investigate biological molecules is unusual but could provide interesting information on metal-ligand vibration and on the conformational state of the molecules. This latter aspect could constitute an important crosslink with the research activities developed by Team 1. The team will continue studies in electrochemistry as well, to monitor electrochemical properties of proteins, eventually coupling the technique with infrared spectroscopy.

The research strategy and the choice of the subjects are interesting and relevant.

- ### Conclusion:

The Team 3 is a small but excellent team, which has developed a specific position in the foreground of the research. Its activities and notoriety are expected to grow and to assess the leadership of its principal investigator. Additional permanent staff hiring should be programmed, both for research and technical support, in particular to interact with the other teams of the research unit. The collaborations and contract activities should be maintained and implemented, to ensure a stable financial support to the research and a strong network of relationships.

Team 4: Spectrométrie de Masse des Interactions et des Systèmes

Team leader: Ms Emmanuelle LEIZE-WAGNER

Workforce

Workforce	Number on 06/30/2011	Number on 01/01/2013	2013-2017 Number of producers**
N1: Professors or assistant professors	1	1	1
N2: EPST or EPIC researchers	2	3	3
N3: Other professors and researchers	1	1	1
N4: Engineers, technicians and administrative staff * on a permanent position	0,3	1	
N5: Engineers, technicians and administrative staff * on a non-permanent position	1		
N6: Postdoctoral students having spent at least 12 months in the unit	1		
N7: Doctoral students	3		
N8: PhD defended	1		
N9: Number of Habilitations to Direct Research (HDR) defended	0		
N10: People habilitated to direct research or similar	2	3	
TOTAL N1 to N7	**9,3**	**6**	**5**

* If different, indicate corresponding FTEs in brackets.

** Number of producers in the 2008-2011 period who will be present in 2013-2017.

• Detailed assessments

Assessment of scientific quality and production:

The group composed by 3 permanent staff (2 CNRS researchers, 1DR2, and 1CR1; 1 assistant professor), 6 PhDs and 1 engineer (employed on contract), was created in January 2008. An emeritus researcher (DRCE CNRS), joined this small unit in January 2011.

Research fields of investigation were axed to:

- the development of mass spectrometry methodologies using ESI-MS (Electrospray Ionisation Mass Spectrometry) and MALDI-MS (Maldi Assisted Laser Desorption Ionization Mass Spectrometry) for the study of supramolecular systems in chemistry and in biology (protein complexes) with the aim of determining the weight, the stoichiometry, and the stability of such complex structures;

- the study of membrane proteins using CE-MS-MS coupling using on-line CE/ESI-Q-TOF and off-line CE/MALDI-TOF-TOF sources and including proteomics approaches (gel multi-enzymatic digestions with different proteases or mixtures ofthem).

Developed by only few laboratories in France, these couplings are especially demanding. The group is notably the European referent of two industrial partners (Bruker Daltonique and Beckman-Coulter) for such instrumental development.

Both goals are great challenges. Through several national and international collaborations involving chemists, biologists and instrument constructors, this group has developped a high level research including a significant risk factor.

The scientific production over 2007-2011 amounts in 19 papers in peer-reviewed journals, 8 invited talks and 17 oral and poster communications, with one PhD defended. All the members are producers and publish in diversified journals with various impact factors. The past and current work more specifically related to the development of the couplings would deserve to be published in journals more connected to the mass spectrometry community and with stronger impact.

Assessment of the research team's integration into its environment:

The team skills are well appreciated by the partners and collaborators of the "Esplanade" site of UDS within the platform of the UMR 7177 (and to a lesser part those of the IBMC). This group has strongly contributed to obtain funds to equip this platform on the basis of (i) successful applications to calls (yielding acquisition of two mass spectrometers - MALDI TOF-TOF and ESI-Q-TOF - part of the maintenance and of the management of which is insured by group members, or (ii) own credits (ANR contracts and development contracts with companies; to acquire several devices - nanoLC chromatography, capillary electrophoresis, purification and desalting systems, ….).

This platform is "vital" for the research activities of the team. Access and modalities of use will have to be well defined to maintain the group activity. The corresponding agreement will allow the group to stabilize and enlarge its network of academic and industrial collaborations, making possible to finance research in terms of non permanent staff (post-docs, IE under contract) and equipments (570 000 € over 4 years).

Assessment of the research team's reputation and drawing power:

Due to their status, the researchers have a weak participation in the teaching programs of the University but are involved, since 2005, in an International Research Training Group (GRK 53), which makes it possible to recruit PhDs, post-docs and researchers within German and French laboratories with which they collaborate.

Assessment of the strategy and 5-year project:

The project is centered mainly on four lines linked to mass spectrometric techniques: (i) Development of methods to analyze the nucleation processes of non-covalent complexes; (ii) Development of methodologies to characterise membrane protein complexes (cross-linking strategies and analysis by proteomics); (iii) Development of a rapid and complete high resolution characterisation method of intact isoform proteins with capillary electrophoresis–MS interface; (iv) Study of proteins extracted from archaeo-materials (involving a new incoming assistant professor). These themes of research will be addressed in the continuity of the current work but more in connection with internal collaborations in the new unit.

The feasibility of this project depends on two main points: (i) the methodology of analysis of complex or even very complex systems (membrane proteins); (ii) the CE-MS-MS couplings, of technological order. This project is not really original (numerous groups work on such analytical challenges) but presents a real risk-taking. The success will depend mainly on the availability of equipment (machine time of the analytical platform) and even of new purchases considering that the new CESI interface (200 k€) is loaned during 18 months by Beckman-Coulter.

Conclusion:

This team has demonstrated its strong expertise and its skills to approach analytical challenges by mass spectrometric techniques and capillary electrophoresis, and its capacity to look for financing. Within the new unit, it will be definitively able to develop interactions with other groups by using complementary approaches. It benefits from (i) a specific partnership with the proteomic platform of IBMC, Strasbourg; (ii) strong collaborations with industrial partners (Bruker Daltonique and Beckman-Coulter) which can provide an important support for new technological developments; (iii) several national and international collaborations. In contrast, it has limited autonomy since it heavily relies on platform equipments. From the latter point of view, some specific agreement must be established in relation to the equipments of the scientific platform of the federative structure presently managed by the UMR 7177. Moreover the team projects are ambitious and difficult with respect to the number of permanent staff. Efforts should be concentrated without multiplying applications (at the risk of appearing as just a service provider).

Team 5:	Chemoinformatique
Team leader:	Mr Alexandre VARNEK

Workforce

Workforce	Number on 06/30/2011	Number on 01/01/2013	2013-2017 Number of producers**
N1: Professors or assistant professors	2	2	2
N2: EPST or EPIC researchers	1	1	1
N3: Other professors and researchers	0		
N4: Engineers, technicians and administrative staff * on a permanent position	0		
N5: Engineers, technicians and administrative staff * on a non-permanent position	0		
N6: Postdoctoral students having spent at least 12 months in the unit	4		
N7: Doctoral students	7		
N8: PhD defended	3		
N9: Number of Habilitations to Direct Research (HDR) defended	1		
N10: People habilitated to direct research or similar	2		
TOTAL N1 to N7	**14**	**3**	**3**

* If different, indicate corresponding FTEs in brackets.

** Number of producers in the 2008-2011 period who will be present in 2013-2017.

• Detailed assessments

Assessment of scientific quality and production:

Team 5 is constituted by one professor, one "directeur de recherche" CNRS and one assistant professor. The central activity of this group is to develop new theoretical descriptions of molecular systems in order to propose new ways to analyze their properties. To this end, the team refines some theories and their domain of applicability but also produces new software.

For the period of reference, the team has produced an important number of papers (41). This corresponds to an average of 3.2 papers per permanent and per year. These articles have been published beyond the framework of the team and articles written in collaboration have led to publication in multidisciplinary journals. Members of the team have also participated to 5 books on Chemoinformatics, have given more than 50 conferences and have also taken part to the organization of 14 international symposia, workshops and summer schools.

The scientific production and the dynamism of this team make it a national and international reference in the field of Chemoinformatics.

- ### Assessment of the research team's integration into its environment:

Overall, the team has proved its capability to obtain funding from various sources. The group has been successful with respect to applications to local and national calls (Region, CNRS, MAE, ANR) but has also received funds from the EU. Moreover, it has established several contracts with private companies quite exclusively through collaborative researches. This aspect of valorization is also attested by the realisation of numerous programs derived from their research that can be now used by any researcher interested by this field. The team is also notably involved in training at the Master level, both at national and international level.

Assessment of the research team's reputation and drawing power:

During the period of reference, the team has received an important number of invited researchers (13; including 5 for periods longer than three months), all of them from abroad, and has hired 4 post-doctoral associates. The group leader is also the coordinator of two "Groupement de Recherche", one national in Chemoinformatics, one international in supramolecular chemistry. These points underline the existence of well-established and long-lasting collaborations with several laboratories in France and abroad.

Assessment of the strategy and 5-year project:

The team has proposed a relevant project, both as a continuity of the existing research but also as an innovative evolution of the axes developed nowadays. Two main directions concern new aspects of the theoretical descriptions of molecular compounds and chemical reactions as well as investigations of 2D and 3D interactions between molecular systems. For each aspect of this project, a detailed overview of the needs (both technical and human) but also of the engaged collaborations is presented, attesting the feasibility of the project on a medium- and long-term. In agreement with the "Directoire" of the new UMR, the team exposed its policy in term of development. This team stressed its wish to create new collaborations within the new laboratory.

In summary, the strategy of this team concerning its project and development seems very relevant.

Conclusion:

This team has become a national and international reference in the field of Chemoinformatics and the projects should strengthen its excellent positioning. The contract activities should be maintained in order to obtain enough funds to allow a technical development as well as to guarantee continuity in the collaborations with foreign groups. Additional permanent staff hiring should be programmed, mainly for technical support that could first stabilize and then enhance the development of new softwares. Establishment of strong collaborations with members of the other teams of the new unit is a good opportunity to access to multidisciplinary and high-impact publications.

5 ● Grading

Once the visits for the 2011-2012 evaluation campaign had been completed, the chairpersons of the expert committees, who met per disciplinary group, proceeded to attribute a score to the research units in their group (and, when necessary, for these units' in-house teams).

This score (A+, A, B, C) concerned each of the four criteria defined by the AERES and was given along with an overall assessment.

With respect to this score, the research unit concerned by this report (and, when necessary, its in-house teams) received the overall assessment and the following grades:

Overall assessment of the unit : Chimie de la matière complexe - CMC

Unité dont la production, le rayonnement, l'organisation, l'animation et le projet sont très bons.

Grading table:

C1 Scientific quality and production.	C2 Reputation and drawing power, integration into the environment.	C3 Laboratory life and governance.	C4 Strategy and scientific project.
A	**A**	**A**	**A**

Overall assessment of the team : Tectonique Moléculaire

Équipe dont la production est excellente, le rayonnement et le projet sont très bons.

Grading table:

C1 Scientific quality and production.	C2 Reputation and drawing power, integration into the environment.	C3 Laboratory life and governance.	C4 Strategy and scientific project.
A+	**A**	**-**	**A**

Overall assessment of the team : Chimie Moléculaire du Solide

Équipe dont la production, le rayonnement et le projet sont bons mais pourraient être améliorés.

Grading table:

C1 Scientific quality and production.	C2 Reputation and drawing power, integration into the environment.	C3 Laboratory life and governance.	C4 Strategy and scientific project.
B	**B**	**-**	**B**

Overall assessment of the team : Bioélectrochimie et Spectroscopie

Équipe dont la production est excellente, le rayonnement et le projet sont très bons.

Grading table:

C1 Scientific quality and production.	C2 Reputation and drawing power, integration into the environment.	C3 Laboratory life and governance.	C4 Strategy and scientific project.
A+	**A**	**-**	**A**

Overall assessment of the team : Spectrométrie de Masse des Interactions et des Systèmes

Équipe dont la production et le projet sont bons mais pourraient être améliorés, le rayonnement est très bon.

Grading table:

C1 Scientific quality and production.	C2 Reputation and drawing power, integration into the environment.	C3 Laboratory life and governance.	C4 Strategy and scientific project.
B	**A**	**-**	**B**

Overall assessment of the team : Chemoinformatique

Équipe dont la production, le rayonnement et le projet sont très bons.

Grading table:

C1 Scientific quality and production.	C2 Reputation and drawing power, integration into the environment.	C3 Laboratory life and governance.	C4 Strategy and scientific project.
A	**A**	**-**	**A**

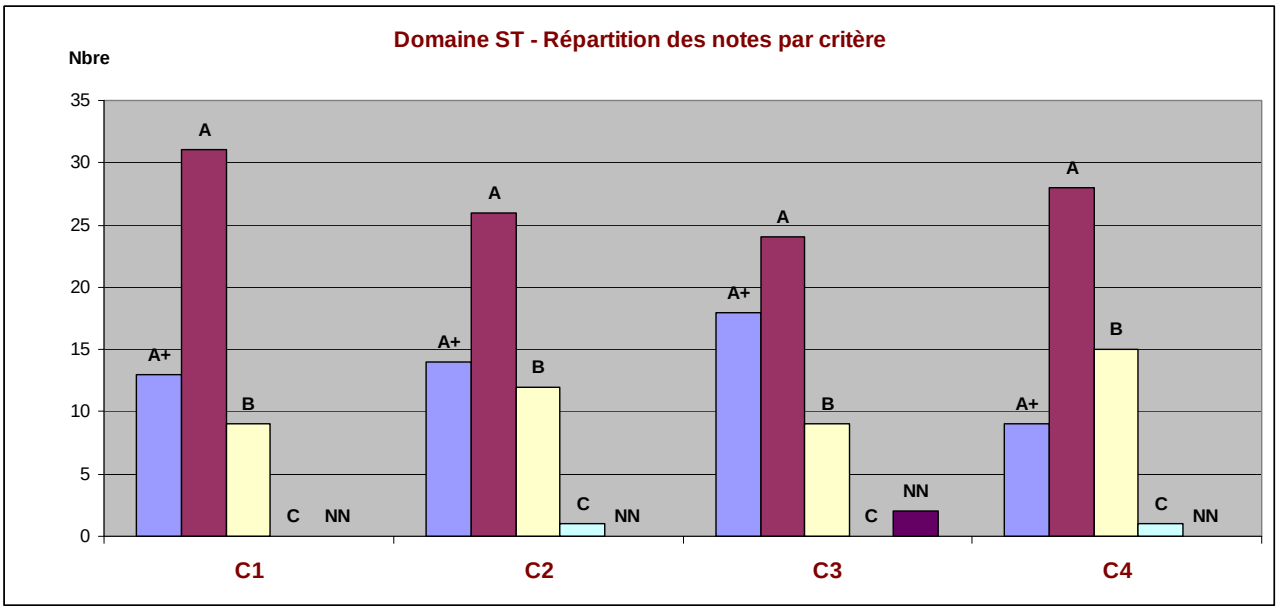
6 • Statistics per field : ST au 10/05/2012

Notes

Critères	C1	C2	C3	C4
	Scientific quality and production	Reputation and drawing power, integration into the environment	Laboratory life and governance	Strategy and scientific project
A+	13	14	18	9
A	31	26	24	28
B	9	12	9	15
C	-	1	-	1
Non noté	-	-	2	-

Pourcentages

Critères	C1	C2	C3	C4
	Scientific quality and production	Reputation and drawing power, integration into the environment	Laboratory life and governance	Strategy and scientific project
A+	25%	26%	34%	17%
A	58%	49%	45%	53%
B	17%	23%	17%	28%
C	-	2%	-	2%
Non noté	-	-	4%	-



7 • Supervising bodies' general comments

UNIVERSITÉ DE STRASBOURG

Monsieur Pierre GLAUDES
Directeur de la Section des Unités de recherche
Agence d'évaluation de la recherche et de l'enseignement supérieur (AERES)
20 rue Vivienne
75002 PARIS

Alain BERETZ
Président

Strasbourg, le 11 avril 2012

Objet : Rapport d'évaluation de l'UMR 7140 « Chimie de la matière complexe » (réf. S2PUR130004524-RT)
Réf. : AB/EW/N° 2012-174

Affaire suivie par
Eric WESTHOF
Vice-président Recherche
et formation doctorale
Tél : +33 (0)3 68 85 15 80
eric.westhof@unistra.fr

Direction de la recherche

Cher collègue,

Je vous remercie pour l'évaluation de l'unité mixte de recherche « Chimie de la matière complexe » dirigée par Monsieur Mir Wais Hosseini.

Vous trouverez ci-joint les réponses du porteur de projet concernant les erreurs factuelles et les remarques et appréciations du comité d'experts.

Je partage l'étonnement du directeur de l'unité quant à la perception négative du comité de visite sur les implications des membres de l'unité dans des activités d'intérêt collectif et à la relation effectuée avec la taille de l'unité. Pour le reste, je n'ai pas de remarque particulière à ajouter au nom de l'Université.

Je vous prie d'agréer, Cher Collègue, l'expression de mes sentiments distingués.

Alain BERETZ

P.J. :

- **Une première partie corrigeant les erreurs factuelles**
- **Une seconde partie comprenant les observations de portée générale**

4 rue Blaise Pascal
CS 90032
F-67081 STRASBOURG cedex
Tél. : +33 (0)3 68 85 15 80
Fax : +33 (0)3 68 85 12 62
www.unistra.fr

Commentaires sur le compte rendu d'évaluation de l'UMR 7140

La disparité et l'inhomogénéité des critères d'analyse et d'appréciations, perceptibles à la lecture du rapport, donne une image brouillée de la complémentarité et de la dynamique de l'unité. Ainsi les critères comme le nombre de publication normalisé par rapport au nombre de publiants, les citations sur la période considérée, les conférences et séminaires, les modes de financement etc, ne sont ni considérés ni analysés de la même façon pour les différents groupes de recherche.

Le comité d'évaluation met en exergue de façon ostentatoire une faiblesse estimée des aspects applicatifs des recherches menées ce qui semble une conséquence inévitable du caractère fondamental et original de telles recherches. Même si nous considérons que le transfert vers l'appliqué est indéniablement intéressant et un plus, mener des recherches à caractère fondamental est certainement l'une des missions de la recherche publique et universitaire. Cet aspect ne devrait sans doute pas être considéré dans l'absolu de façon négative mais évalué au regard du type ou du domaine de recherche.

Concernant la participation à la vie collective et au bon fonctionnement des institutions, au cours d'une réunion organisée par l'Université de Strasbourg, les responsables de l'AERES au plus haut niveau ont très clairement exprimé l'importance donnée à ces taches et l'intérêt à les préciser pour la clarté de d'évaluation. Or dans le rapport, cet aspect est systématiquement présenté de façon négative (faiblesse). Il est à remarquer que les responsabilités assumées par les membres de l'unité relèvent de nominations nationales ou d'élections ouvertes à tous, ce qui dans les deux cas, témoigne d'une reconnaissance nationale ou locale forte. Enfin, les personnes assumant ces responsabilités n'ont abandonné ni l'enseignement ni la recherche et ont publié des manuscrits dans des journaux de très haut niveau. Cette remarque, injustifiée à notre avis, est décourageante et nous apparaît comme un signe très négatif vis-à-vis de l'implication au service de la communauté scientifique.
A l'heure où le ministre de l'enseignement supérieur, à l'occasion de la signature de l'IDEX à Strasbourg, a souligné l'investissement collectif, félicité et remercié ceux qui se sont fortement impliqués pour la réussite de l'ensemble des projets, ces remarques générales paraissent assez curieuses…