

EVALUATION REPORT OF THE UNIT
ISIS - Institut de science et d'ingénierie
supramoléculaires

UNDER THE SUPERVISION OF THE
FOLLOWING ESTABLISHMENTS AND
ORGANISMS:

Université de Strasbourg
Centre National de la Recherche Scientifique -
CNRS

EVALUATION CAMPAIGN 2022-2023
GROUP C



In the name of the expert committee¹ :

Roeland Nolte, Chairman of the committee

For the Hcéres² :

Thierry Coulhon, President

Under the decree n° 2021-1536 of 29th November 2021:

¹ The evaluation reports "are signed by the chairperson of the expert committee". (Article 11, paragraph 2);

² The president of the Hcéres "countersigns the evaluation reports established by the expert committee and signed by their chairperson." (Article 8, paragraph 5).

This report is the result of the unit's evaluation by the expert committee, the composition of which is specified below. The appreciations it contains are the expression of the independent and collegial deliberation of this committee. The numbers in this report are the certified exact data extracted from the deposited files by the supervising body on behalf of the unit.

MEMBERS OF THE EXPERT COMMITTEE

Chairperson:	Mr Roeland Nolte, Radboud University in Nijmegen, The Netherlands
	Ms Chantal Andraud, ENS Lyon
	Mr Peter Chen, Eidgenössische Technische Hochschule, Zürich, Suisse
	Mr Yannick Coppel, CNRS Toulouse (research support personnel)
Experts:	Mr Antonio Echavarren, Institute of Chemical Research of Catalonia, Tarragona, Spain
	Ms Muriel Hissler, Université Rennes 1 (representative of the CNU)
	Mr David Kreher, Université Paris Saclay (representative of the CoNRS)
	Ms Giovanna Morigi, Saarland University, Saarbruecken, Germany
	Mr Stéphane Pellet-Rostaing, Université de Montpellier

HCÉRES REPRESENTATIVE

Mr Henri Cramail

CHARACTERISATION OF THE UNIT

- Name: Institut de Science et d'Ingénierie Supramoléculaires
- Acronym: ISIS
- Label and number: UMR 7006
- Number of teams: 12 teams
- Composition of the executive team: Mr Paolo Samori

SCIENTIFIC PANELS OF THE UNIT

ST Sciences and technologies
ST4 Chemistry

THEMES OF THE UNIT

Research groups at ISIS work on the following themes at the interfaces of chemistry, physics, and biology:

- Supramolecular chemistry (Prof. Jean-Marie Lehn);
- Quantum physics (Prof. Guido Pupillo);
- Nanostructures (Prof. Thomas Ebbesen);
- Supramolecular biomaterials (Prof. Luisa De Cola);
- Chemical catalysis (Prof. John Moran);
- Protein Chemistry (Prof. Vladimir Torbeev);
- Nanochemistry (Prof. Paolo Samori);
- Nonequilibrium complex systems (Prof. Thomas Hermans);
- Complex systems in synthesis and catalysis (Dr. Pawel Dydio);
- Catalytic chemical synthesis (Prof. Amir Hoveyda);
- Exotic quantum matter (Prof. Shannon Whitlock);
- Molecular function and design (Dr. Marco Cecchini).

HISTORIC AND GEOGRAPHICAL LOCATION OF THE UNIT

ISIS is a research institute of the University of Strasbourg and the French National Centre of Research (CNRS) and was founded in 2002 following a blueprint designed by Prof. Jean-Marie Lehn. Its aim is to conduct research in chemistry at the interfaces with physics and biology, focusing on complex matter, which is studied and analyzed by supramolecular approaches. The institute is an international center integrated in the dynamic scientific environment of the upper Rhine on the Strasbourg campus. It is strategically located on the Esplanade Campus in Strasbourg, which also hosts the Faculties of Chemistry, Physics, and Life Sciences.

RESEARCH ENVIRONMENT OF THE UNIT

ISIS aims at opening new fields of research of high scientific and technological relevance. This has made it possible to initiate new sub-fields of chemistry, such as supramolecular chemistry (area of research of Nobel prize winner Prof. Jean-Marie Lehn), chemistry of complex systems, catalysis, chemistry of non-equilibrium systems, strong coupling between light and matter, and multi-responsive materials and devices. More recently a link was made with quantum computing. In the last decade ISIS has been very active within the "Initiative d'Excellence", where it initiated the labex project "Chimie des Systèmes complexes" (CSC) and participated in the labex project "Nanostructures en Interaction avec leur Environnement" (NIE). Both these projects are managed by the organization icFRC, which was also founded by ISIS researchers. According to the self-assessment document ISIS is involved in two equipex projects, i.e. since 2014 as partner in the project "Optique ultrarapide, Nanophotonique et Plasmonique" and since 2021 as coordinator of aQCess, which is a project in the field of quantum physics. ISIS is part of the Chemistry Federation Le Bel, which was created together with CNRS and the University of Strasbourg. This federation includes three research units in chemistry (including ISIS) and an analysis platform. The various groups of ISIS have long-lasting collaborations with academic and industrial groups, both inside and outside of France. All PIs are active in publishing their work and protecting it via patenting, showing that they have a great interest in sharing and exploiting the results of their studies with society. They are also acting frequently as consultants for public and private organizations. ISIS contributes significantly to the training and teaching of students. In this connection, the institute participates in numerous European actions, like the Marie Skłodowska-Curie and the ITN ULTIMAT networks. ISIS is steering the International Graduate School in Complex Systems Chemistry (CSC-IGS), which offers to talented national and international students on the master and Ph.D. level an innovative training on the topic of chemistry of complex systems. It is also involved in another doctoral training program, named Quantum Science and Technologies at the European Campus (QUSTEC), set up by the European Grouping of Territorial Cooperation EUCOR (Upper Rhine network) in collaboration with IBM and funded by the European Union.

UNIT WORKFORCE: in physical persons at 31/12/2021

Permanent personnel in active employment	
Professors and associate professors	5
Lecturer and associate lecturer	1
Senior scientist (Directeur de recherche, DR) and associate	1
Scientist (Chargé de recherche, CR) and associate	5
Other scientists (Chercheurs des EPIC et autres organismes, fondations ou entreprises privées)	0
Research supporting personnel (PAR)	20
Subtotal permanent personnel in active employment	32
Non-permanent teacher-researchers, researchers and associates	11
Non-permanent research supporting personnel (PAR)	15
Post-docs	39
PhD Students	58
Subtotal non-permanent personnel	123
Total	155

DISTRIBUTION OF THE UNIT'S PERMANENTS BY EMPLOYER: non-tutorship employers are grouped under the heading "others".

Employer	EC	C	PAR
CNRS	0	6	11
Université de Strasbourg	6	0	9
Total	6	6	20

UNIT BUDGET

Recurrent budget excluding wage bill allocated by parent institutions (total over 6 years)	1 837
Own resources obtained from regional calls for projects (total over 6 years of sums obtained from AAP idex, i-site, CPER, territorial authorities, etc.)	4 152
Own resources obtained from national calls for projects (total over 6 years of sums obtained on AAP ONR, PIA, ANR, FRM, INCa, etc.)	9 052
Own resources obtained from international call for projects (total over 6 years of sums obtained)	22 874
Own resources issued from the valorisation, transfer and industrial collaboration (total over 6 years of sums obtained through contracts, patents, service activities, services, etc.)	978
Total in K€	38 893

GLOBAL ASSESSMENT

ISIS is a top-ranking research institute, which stands alone in the French scientific landscape. It can compete with the best institutes in Europe and the world. The research carried out by its staff is outstanding in many aspects: the ideas are very creative and innovative, the studies are of very high quality, and the results are published in many articles in top-tier journals, receiving very high citations. Without exception each of the individual laboratories in the fields of chemistry and physics is among the best in its field. The staff of ISIS has been able to raise substantial funding for its research activities, i.e. 4-8 million euro per year. Most of this funding comes from outside France based on public and private research contracts won by its staff and less from France (University of Strasbourg, CNRS, ANR). At its start in 2002 ISIS aimed at developing the highest level of multidisciplinary research at the interfaces of chemistry, physics and biology, with a special focus on the use of supramolecular approaches to the understanding of complex matter. During the last evaluation period ISIS has continued to implement this scientific policy. The research activities in the field of chemistry have been expanded to now include catalysis as well and the interface with physics has been strengthened by establishing links with the "Centre Européen de Sciences Quantiques" (CESQ), which is excellent. The research activities at the interface of chemistry and biology are lagging behind. Currently, there is only one group working on bio-related themes, i.e. a group led by a junior team leader, and that is too little. It is recommended to reconsider this policy and strengthen the chemistry-biology interface with the hiring of new staff, particularly senior ones, which can take the lead in this process of strengthening. The scientific staff of ISIS is composed of few permanent staff and many young scientists. This type of organization is unique in France and has shown to be very successful in the past. In the past evaluation period quite some staff members have left ISIS, perturbing the demographic (age) balance negatively. It is recommended to pay attention to this issue, as it may become a threat for the future. The overall gender balance ratio in science is ca 2:1 (men-women), which is acceptable. Unfortunately, there are no female senior team leaders (Prof. De Cola has left ISIS) and there is only one recently hired female junior team leader, which is a highly undesirable situation. ISIS should also be an institute where talented senior female researchers feel at home, acting as role models for young female scientists. This issue needs attention. The number of supporting administrative and technical staff at ISIS is too low. The expansion of ISIS with ISIS-2 and CESQ, the presence of more technical platforms, and the arrival of new groups has increased the pressure on this staff, which should be diminished by hiring more personnel. This is also important for keeping safe working conditions in the laboratories. The understaffing of administrative and technical personnel should be discussed urgently with the supervising bodies to find a solution. The institute has been excellently managed by the director and his team. With the recent expansion of ISIS, the number of tasks has increased, and the appointment of a suitable new director is a very urgent and important matter. ISIS is very active in the translation of the results of its scientific studies to society and industry, which is excellent. The in-house presence of an industrial department is very instrumental in this and has resulted in many new patents and the establishment of start-up companies, which is very positive. The activities of the institute in bringing its science to the general public is praiseworthy and sets an example for other institutes in France.

DETAILED EVALUATION OF THE UNIT

A - CONSIDERATION OF THE RECOMMENDATIONS IN THE PREVIOUS REPORT

1. *Assessment of scientific quality and outputs*

The previous evaluation report was very positive about the quality of the research at ISIS and about the output of scientific papers, which were published in high profile journals. No weakness was found, and the institute was called a gemstone not only in the French landscape, but also in the arena of international science. It was recommended to continue with the same enthusiasm. In line with this, in the past period the institute further strengthened its scientific position by starting new activities in the fields of catalysis and quantum computing. To facilitate this ISIS has been expanded with two new buildings: ISIS-2 and the "Centre Européen de Sciences Quantiques" (CESQ).

2. *Assessment of the unit academic reputation and appeal*

With the high number of Nobel laureates in the institute, the impressive number of awards the team leaders had received in the previous evaluation period, and the ability of the institute to raise substantial amounts of funding for research, the academic reputation of ISIS was evaluated to be excellent. No change was found to be necessary.

3. *Assessment of the unit interaction with the social, economic and cultural environment*

The interaction of the institute with the social, economic and cultural environment was excellent in all aspects, i.e. the collaboration with industry (ISIS houses laboratories of several large industrial companies), the creation of start-up companies, and the organization of events where the general public can meet scientists and hear about their work. The recommendation was to continue in the same way and stay on course towards excellency.

4. *Assessment of the unit organization and life*

With respect to the assessment of this aspect the previous evaluation report gave some recommendations. It was noted that the organization of ISIS is operating with a limited number of permanent staff and many non-permanent young scientists, which is unique in France. Junior team leaders can only stay for 6 years and then must move to positions elsewhere in Strasbourg and in France. New junior team members are selected by the "Directoire", a board composed of an international committee which comprises ISIS PIs senior and high caliber international scientists. Each research team is independent with respect to its financial management and scientific organization. The previous evaluation report felt that the number of permanent support staffs at ISIS was subcritical and this might become a problem if the institute further expands, as not enough technical staff would be available to run the new equipment. Also, the financial staff might not be able to manage the funding contracts that were expected to further increase when the institute becomes larger. The report recommended to ask for more permanent positions in the IT and scientific equipment management to avoid critical administrative, technical and logistical understaffing. The latter would make that tasks have to be allocated to scientists, which is undesirable. The self-assessment report reveals that the number of supporting staffs has not increased much in the period 2016-2021, in deviation from what was recommended. This issue remains critical and requires attention.

5. *Assessment of the unit involvement in training through research*

The institute trains numerous doctoral and master students and the qualities of the guidance and supervision were evaluated to be very good. The students were also involved in international training programs (Erasmus, ITN). There are monthly seminars where young scientists give presentations about their work, but not everybody gets a turn. The previous report recommended to organize an annual doctoral student day with short presentations and poster sessions, allowing everybody to show her/his work. The self-assessment document does not indicate whether this suggestion has been implemented by the institute, but enquiries with the director revealed that the faculty takes care of this. The previous report furthermore asked for a further clarification of the general policy of the institute with respect to the participation of PhD students in national and international conferences. This clarification has not been given in the report over the period 2016-2021. However, the director indicated that all Ph.D. students are supposed to participate in international conferences and that this is stimulated by the supervisors.

6. Assessment of the strategy and the five-year plan

ISIS planned an extension of the building and an increase in the number of research groups in their five-year plan. This plan has been realized in the past period. A beautiful new wing (ISIS-2) has been added to the existing building and new groups in chemistry and physics have made their entrance into ISIS.

B – EVALUATION AREAS

EVALUATION AREA 1: PROFILE, RESOURCES AND ORGANISATION OF THE UNIT

Assessment on the unit's resources

ISIS is a unique institute in France. Because of its excellent scientific performance, the authorities have provided the resources for a new wing (ISIS-2) to the existing premises and for the establishment of the "Centre Européen de Sciences Quantiques" (CESQ). ISIS-2 now houses new top research groups that are focusing on catalysis research. In the last evaluation period ISIS has been able to attract substantial funding for its research activities, amounting 4-8 million euro per year, which is excellent. This funding comes from three sources: University of Strasbourg and CNRS, public and private research contracts, and internal resources of the institute itself. With this money, it has been able to create a great research environment, characterized by a very high research activity. A great danger for the future is the technical and administrative understaffing of the institute. This will force scientists to perform tasks for which they have not been appointed. This critical issue should be resolved as soon as possible.

Assessment on the scientific objectives of the unit

ISIS is a top institute, which was created in 2002 following a blueprint by Prof. Jean-Marie Lehn. The scientific objectives of the institute are clearly formulated. Its scientific performance is outstanding, and the institute is very visible and has a very high international status. It is currently one of the leading institutes worldwide. Over the years, ISIS has rejuvenated itself several times, most recently again by taking a focus on catalysis and by embracing quantum computing as new direction of research. A weakness and possible risk for the future is the fact that the interface with biology is not very well developed. This is not in line with the original principles of the institute and requires further attention. A forward-looking policy on this aspect is lacking.

Assessment on the functioning of the unit

ISIS has an organization that is flexible, leaving a lot of responsibilities to the scientific team leaders. The human resources are adequately managed, although a general plan on how to hire and keep the best staff is lacking. The overall gender balance of the institute is acceptable, but the number of female senior and junior team leaders is far too low. This issue should be addressed as soon as possible. The director manages the institute very well and the report shows that the scientific assets of ISIS are well protected. Although a local health, safety and working conditions committee (CLHSCT) has been created, safety remains an issue of concern. The institute has not enough technical support staff that can help, together with the group leaders, create safe working conditions.

1/ The unit has resources that are suited to its activity profile and research environment.

Strengths and possibilities linked to the context

The structure of ISIS is unique in France as it is composed of a limited number of permanent staff and many non-permanent young scientists, which are the active players in various research projects. This operating mode makes it possible to respond quickly to new scientific developments. Two notable events in the last period are the link ISIS has made with the European Center for Quantum Sciences (CESQ) and the recent focus of the

institute on catalysis. For the latter a new wing has been added to the ISIS building (ISIS-2), which now houses amongst others the laboratories of Catalytic chemical synthesis and Chemical catalysis. This wing was opened in October 2019 and has enlarged ISIS by 2200 m², which is appreciable. The financial resources for this extension were provided by the program “Opération Campus”, initiated in 2009 by the State. Worth mentioning is also that in 2019 ISIS has established so-called Associated laboratories, which are expected to further enhance the research profile of the institute. The funding of ISIS comes from three different sources: (i) yearly recurring credits from the University of Strasbourg and CNRS; (ii) public and private research contracts obtained by the team leaders; and (iii) internal resources of the institute itself. The resources from the University of Strasbourg and CNRS have remained roughly constant over the years. The research contracts are appreciable and amount to circa 4-8 million euros per year. From each contract a small sum (3.15%) is taken to enable the purchase and maintenance of common equipment. Funding for the installation of new teams can also come through the submission and evaluation of proposals from the International Center for Frontier Research (IFRC). Private companies wishing to start a research department at ISIS also bring in internal revenues. ISIS pools part of its own funds to promote collective research activities and to initiate new research themes. One-third is redistributed to the research teams in proportion to their size, a second third is used for operational issues (e.g. security and reconstruction costs of the premises), and the last third is set in to support collective research activities, the maintenance of equipment, and costs related to the overall functioning of the institute. The conclusion is that the institute has been able to raise substantial funding for its research activities and the training of young scientists, which is excellent. This funding is used to create a very inspiring research environment and to further shape the research profile of the institute. The latter makes the institute very visible on the national and international platforms, allowing it to attract top scientists and to make strong links with industry.

Weaknesses and risks linked to the context

The committee noticed that quite some PIs have left ISIS in the past period and another PI will leave next year. These resignations disturb the age balance of the institute and makes it fragile. This issue needs attention. According to the documents the technical and administrative staff of ISIS is minimal, i.e. their number compared to the number of people working at ISIS is only 10%. This is a serious threat for keeping the high quality of the institute in the future. The recent extension of ISIS with a new wing and the link that has been established with the CESQ center make this problem even more serious. The resources for the support staff come from the University of Strasbourg and CNRS and are negotiated annually. These resources should be increased considerably. The logistic team is composed of only two permanent and one non-permanent employees, which are responsible for the logistic and technical support as well as the safety in three buildings covering an inner surface of over 15.000 m². This is an unacceptable situation, which should change rapidly. The more so as it is a serious threat to safety as well. Without more help the scientific staff will be forced to step in themselves and this is detrimental to their research activities. The same holds for the administrative support staff. Since 2016 only 4 assistants have done all the administrative work. At the end of 2021, a 5th assistant has joined ISIS, but this is far from adequate for the future, because the institute has expanded considerably with new research groups bringing in many new contracts. The complexity of managing the large number of private and public contracts and the fact that several PIs are coordinator of international projects in European programs exceed the capabilities of the current administrative staff and this situation should be changed rapidly. The low number of permanent scientific and technical/administrative staff is detrimental to ISIS as it also makes that less funding will be obtained from “Agence Nationale de la Recherche” (ANR), which favors institutes and laboratories with a high number of permanent staff. The above analysis is in line with the distribution credits of ISIS’ resources shown in the self-evaluation report on page 13. In the period 2018 to 2021, the allocation of funds to the teams has decreased from 31 to 19% and the available money for equipment and safety from 30 to 19%. This reallocation was needed to balance the costs of administrative and logistic tasks, which increased from 22 to 41%. This illustrates the urgency of the situation. The new wing of ISIS and the CESQ center are important for the new scientific activities of the institute. It is not clear from the self-evaluation document how the maintenance and the guardianship of the new buildings are organized, but according to a representative of the university present at the site visit, the University of Strasbourg will ensure this.

2/ The unit has set itself scientific objectives, including the forward-looking aspect of its policy.

Strengths and possibilities linked to the context

ISIS was founded in 2002 based on a blueprint designed by Prof. Jean-Marie Lehn. It aims at developing and promoting the highest level of multidisciplinary research at the interfaces of chemistry, physics and biology, focusing on supramolecular approaches to the understanding and manipulation of complex matter. Since its start the institute has grown in scientific quality, status, and visibility. It is now probably the leading research institute in France and of comparable quality as the leading research institutes in Europe and the world, e.g. the Medical Research Center in Cambridge, UK, some of the Max Planck institutes in Germany, and the Scripps Research Institute in California, USA. The research carried out by the various groups is very creative, highly

imaginative and bold with respect to the proposed new concepts and ideas. The productivity is extremely high, both in terms of quality and quantity of the published papers. The past years have shown that the model of ISIS is probably the best possible investment in science one can think of. The institute also benefits the national economy of France by training top scientists, by transferring knowledge to industry, by creating spin-off activities, and by advertising France as a leading country in science in Europe and the world. ISIS rejuvenates itself again and again by taking new directions and by setting new scientific targets. An example is the new focus of the institute on catalysis. By hiring two new top scientists from the United States, including a Nobel Prize winner, ISIS has shown to have a clear scientific vision. Catalysis is crucial for industry and society and this new focus guarantees that in the future new exciting catalytic systems, very much comparable to the efficient biocatalytic systems found in Nature, will be developed. The close connection of the institute with industry (many leading European industries have departments at ISIS) will facilitate the efficient transfer of this knowledge in catalysis to companies, creating a high economic value for society. A second example of the excellent vision of the institute is the embracing of quantum computing. For this, recently, a firm connection has been made with the new European Center for Quantum Sciences. New ways of computing and storing of information are essential for society given the current enormous increase in data generation, which subsequently must be stored and processed (artificial intelligence is an example). Chemical ways of thinking on how to handle complex systems will be of great help to further develop the world of quantum computing.

Weaknesses and risks linked to the context

At the start of ISIS, it was decided to focus the research of the institute on complex systems at the interfaces of physics and biology, which was an excellent idea. With the hiring of Prof. Thomas Ebbesen in 1999, the link with physics was realized and new directions of research were taken, leading to magnificent scientific discoveries at the interface of chemistry and physics. This physics connection has been further strengthened recently with the recent embracement by ISIS of the European Center for Quantum Sciences. This new connection can be expected to result in new exciting and unexpected developments, fully in accordance with the original blueprint of the institute. A disadvantage is that the center is located at the Cronenburg campus, which may be a risk for integration to ISIS and the creation of research connections with its laboratories. The self-assessment document shows that the link with biology has not been strengthened equally well in the past period. There was only one senior group leader active within ISIS at the interface with biology, heading the Laboratory of protein chemistry, and this person has left ISIS in 2020. Fortunately, at the end of 2021 a new female junior team leader was hired, and she has started the Laboratory of supramolecular biochemistry. Given the importance of the fields of chemical biology and synthetic biology and the enormous challenges today in these fields this limited activity at the interface with biology is a weakness and a risk for the future. The new female team leader has no sparring partners and a senior scientist active in the chemical or synthetic biology field would be highly desirable. This area of research is of great importance to society and may lead to important connections with industry as well. Such an extension would be beneficial for ISIS and in line with the initial blueprint of the institute. A possible renewed focus on biology in the future would be part of a more general forward-looking policy plan of the institute. Unfortunately, the self-assessment document does not provide such a plan.

3/ The functioning of the unit complies with the regulations on human resources management, safety, the environment and the protection of scientific assets.

Strengths and possibilities linked to the context

The mode of operation of the institute follows the original blueprint of the institute with research activities focusing on complex matter at the interfaces of chemistry, physics and biology. The committee notes that the organization is flexible and dynamic as it has a low number of permanent senior staff and many non-permanent young scientists. The team leaders are independent and free to choose their own research focus. They manage their research teams in a way fitting them best and they are supposed to raise their own funding. Within this operation mode it is crucial to hire the best scientist according to the highest international standards. This is done by a panel composed of the senior team leaders of ISIS and two external members, which is fine. Openings for Ph.D. students and postdocs are advertised on the website of ISIS and on international science job websites. For hiring the candidates are interviewed, and reference letters are requested. This procedure is efficient and has worked well in the past. The new young researchers are coached during their stay by their supervisors and by administrative assistants. This is an important procedure and essential for their well-being. In general, the permanent staff, researchers and support staff form united teams, which is beneficial for the success of ISIS. Prof. Paolo Samori has been the director of ISIS in two subsequent periods of 5 year. Together with the administrative director Mrs. Muriel Muzet he has done a tremendous job. ISIS has become a large institute and dealing with all the issues is not an easy task for the director. His directorship has not prevented him from being a very successful group leader as well. The well-being of the institute is a priority for the director, and he has put numerous initiatives in place to make the working conditions as best as possible. In this connection, the administrator director organizes weekly meetings with the research teams, which is excellent. He also keeps an eye on the

administrative staff by having regular meetings with them. For the permanent staff, researchers, and technicians the management provides support for the annual promotion applications to the University of Strasbourg and the CNRS. The management also encourages the employees to follow internal and external training courses, which is very good. Bi-monthly meetings are organized in which the administrative, technical, and scientific staff are informed about recent developments. ISIS has taken adequate measures to protect the scientific assets and the computer systems of the institute. Local IT hubs grouped around a geographical site or a scientific theme have been set up by the University of Strasbourg and CNRS, which is excellent. ISIS manages the backup and archiving of rough spectral data. This data and the processed data are archived on the ISIS server and on the server of the IT department of the Federation of Chemistry (FR2010). All researchers keep laboratory journals, which are stored in two archive rooms at ISIS and ISIS-2. All this shows that the protection of the scientific assets is well organized.

Weaknesses and risks linked to the context

The human resource management of ISIS is fine, although some comments must be made. Human capital is the most precious asset of the institute and a clear plan is needed to guarantee that the best staff is hired and stays at the institute. The self-assessment document provides some indications on how the hiring process is organized, but otherwise remains vague, which is a pity. ISIS' diversity is strongly promoted. The institute features 39 staff members and a very large number of Ph.D. students and post-docs, who come from all the world. The report mentions 28 nationalities of which 44 are French and 115 foreigners. The gender balance is 106 men and 53 women, which is acceptable, but not good. Unfortunately, this gender balance is not reflected in the senior and junior scientific staff: there was only one female senior team leader and she has left ISIS in 2020. Until very recently there was no female junior team leader at all. Only at the end of 2021, a new female junior staff member has been hired. This unfavorable gender balance is a great concern and a risk for the future. The committee feels that all efforts should be taken by the senior PIs to correct this omission. A further concern is the safety of the working conditions in the laboratories. As was already mentioned in section 1 (see above) the number of technical staffs at ISIS is unacceptable low. They must spend most of their time on solving instrumental issues, proclaiming, as an unintended consequence, a risk that other activities such as safety, may receive less attention than would be optimal. The report does not clearly indicate how safety is guaranteed, although it is rewarding to read that in December 2019 a local health, safety and working conditions committee (CLHSCT) has been created. Very recently, the "Règlement intérieur" of ISIS has been updated and this document is currently under validation. ISIS has increased in size considerably and concomitantly the number of issues that must be taken care of by the director has become much larger than in the past. For the coming period of 5 years a new director, which replaces Prof. Samori, must be found. The committee wishes the board of ISIS success in finding a person that has scientific and managerial skills equal to those of the current director.

EVALUATION AREA 2: ATTRACTIVENESS

Assessment on the attractiveness of the unit

ISIS has an outstanding scientific reputation, is very visible, and is an excellent place for its staff to do research. It receives substantial funding in competitive calls for grants from Europe, e.g. 11 ERC and 24 Marie Curie grants in the past evaluation period, which is well above the French standards. The working atmosphere for staff and students is excellent and as a result many top scientists have come to ISIS to spend a sabbatical period. With its cutting-edge research activities, many papers in top journals, and the excellent technical facilities ISIS strongly contributes to the European research area. A weakness is that most permanent senior and junior staff are male, which is a threat for the future. The institute must make an extra effort to attract female staff, e.g. by reserving extra funds for female researchers and by launching extra hiring programs. The analytical and technical platforms are modern and up to date and will be integrated in the future in the university, CNRS, and Inserm network of platforms CORTECS, which is excellent. The low number of technical support staff is a serious threat for the future.

1/ The unit has an attractive scientific reputation and contributes to the construction of the European research area.

Strengths and possibilities linked to the context

From its start ISIS has been set up as a top research institute, rivalling other institutes in France and in Europe. Looking back, it has lived up to this. The institute is very visible and attracts the best researchers from all over the world. Its science is very creative, cutting edge, and leads to applications that are useful for society. ISIS is very

dynamic and responds quickly to new scientific developments. An example of this is its recent focus on catalysis and on quantum computing. For these two research areas the institute has been able to attract the best scientists in these fields, which is admirable. The attachment of a new wing with new laboratories to the existing building has created improved working conditions, which will further boost cutting edge science in the future. The presence of many top researchers in one close area is very beneficial for the exchange of ideas and the development of new directions of research. A nice example of this is the collaboration between the chemistry group of Prof. John Moran and the physics group of Prof. Thomas Ebbesen on the modulation of chemical reactions by coupling vibration modes of organic molecules with the vacuum field by means of photonic cavities. This has resulted in papers in top journals. The senior and junior team leaders have been able to attract substantial funding from the European Research Council (ERC) for their activities, showing that the institute contributes strongly to the construction of the European research area. In this connection it is also worth mentioning that in March 2017 the celebration of the 10th anniversary of ERC was held at ISIS in the presence of many officials from Europe and France, including the president of the ERC. ISIS also participated in the organization of the visit of the President of the state Baden-Wuerttemberg in Germany and the Minister for European Affairs, during which the new doctoral training project Qustec, which addresses some of the grand questions in the field of quantum science, was introduced. The PIs of ISIS are frequently invited to give lectures at major international conferences and at universities and institutes all over the world. The report mentions a number as high as 750 lectures, most of them coming to the credits of Profs. Lehn, Sauvage, and Ebbesen. ISIS members are also very active in organizing scientific meetings, which have up to 100 participants. The report summarizes a number of these meetings, which have helped further increase the scientific reputation of ISIS. In the past period many prizes and awards (over 100) were awarded to ISIS members, which confirms the international scientific fame of the institute. In summary, ISIS has a splendid scientific reputation and has created an attractive working atmosphere in which new and unexpected scientific discoveries are made, contributing strongly to the European research area.

Weaknesses and risks linked to the context

ISIS is very attractive to top scientists from all over the world. However, in the past these scientists were nearly exclusively male. As already mentioned in Evaluation area 1, section 3 this is a threat for the future. In order to be attractive for female students and scientists and to act as a role model for them, the institute must develop a new policy for the future hiring of scientific staff. Female top scientist may be invited to give lectures at ISIS and collaborative projects with female professors from other universities should be stimulated and co-funded. Special exchange programs for female Ph.D. students and post-docs may be initiated. This requires additional money, but this will be well spent.

2/ The unit is attractive for the quality of its staff hosting policy.

Strengths and possibilities linked to the context

ISIS is an attractive institute to conduct research on complex chemical systems at the interfaces of physics and biology. Its premises are excellent and have recently been extended. Its scientific staff has the possibility to interact with other top scientists within the institute, which generates new ideas and new directions of research. ISIS houses 4 Nobel prize winners and one Kavli prize winner. This prestige also radiates to the other researchers and is beneficial for them as these senior prize-winning scientists have extended networks, which can be used by them. The staff meets many top scientific researchers from all over the world, which give lectures at ISIS, and this opens possibilities for them to present their own research and to exchange ideas. The institute has an excellent policy to hire the best scientists, allowing them to work out their ideas. Scientists at ISIS are free to formulate their own research directions, and this has paid off in the past. A further positive point is the fact that several European companies have departments at ISIS. This creates strong interactions between fundamental and applied research, creating possibilities to more easily file patents and set up spin-off companies. One of the ambitions of ISIS is to provide young Ph.D. students and postdocs the highest level of training through research in the field of complex systems, preparing them for a career in academia or industry. This new generation of scientists is expected to be ambassadors of the ISIS training model worldwide. The Ph.D. students are also taught soft skills, such as presentation skills, management skills, and entrepreneurship. Many students that were trained at ISIS have now professorships at top universities, as is documented in the report of the institute. During the last 6 years, ISIS has hosted dozens of guest researchers from all over the world, who spend a sabbatical period in the institute. This clearly evidences the excellent hosting policy of the institute. Sometimes partial funding for this was obtained from the USIAS program of the University of Strasbourg.

Weaknesses and risks linked to the context

A weakness is that the institute has very few female senior and junior scientists. Hence, its role model function for women is very limited. This issue has already been discussed above. Another weakness is that the institute cannot provide enough supporting staff for its scientists. This problem has also been mentioned above.

3/ The unit is attractive because of the recognition gained through its success in competitive calls for projects.

Strengths and possibilities linked to the context

The staff of ISIS is very active in raising funds for their projects, i.e. some 4-8 million euros per year. Most of the funding is obtained via competitive calls and the success rate is very high. The report mentions that since 2016 150 research contracts have been awarded to PIs, including 64 European projects of which 11 were ERC grants and 24 Marie Curie grants. This is an excellent score. PIs also act as coordinators of large European networks, such as the Graphene Flagship and the Marie Curie Ultimate training network led by Prof. Samori and the CReaNet project led by Prof. Hermans. Apart from this, ISIS is strongly involved in projects funded by the Future Investments Programs PIA steering initiative. It has initiated the labex on Chemistry of Complex Systems (CSC) program, which focuses on major challenges in the field of supramolecular chemistry as identified by Prof. Jean-Marie Lehn. Prof Thomas Ebbesen has translated his ideas on light-matter interactions and nanoscience in two programs, i.e. labex Nanostructures in their Environment (NIE) and Optique Ultrarapide, Nanophotonique et Plasmonique (UNION). These are great initiatives. Another program coordinated by ISIS is the aQCess project, which is the first public platform for quantum computing in France. Several other initiatives are mentioned in the activity report and the committee is very positive about all these activities.

Weaknesses and risks linked to the context

Unfortunately, ISIS does not attract substantial funding from the National Research Agency (ANR), which is regrettable. According to the self-evaluation report this is a result of the fact that the ANR funding rules are not compatible with the ISIS model, which strives for few permanent staff and many non-permanent scientists. Despite this, 10 projects were funded by ANR, including the project PRACCATAL of Prof. Amir Hoveyda and the aQCess equipex project of Prof Guido Pupillo. Another threat is the low number of graduate students financed by the local and national research authorities. ISIS compensates this by using its contract-based financial resources for this purpose. This model may not be sustainable if the number of grants of PIs drops for some reason in the future. The committee notes that most of the funding of ISIS comes from outside France, e.g. the European Community, and not from France itself. This issue should be analyzed further and discussed with the University of Strasbourg and the CNRS to make the future financially more sustainable.

4/ The unit is attractive for the quality of its major equipment and technological skills.

Strengths and possibilities linked to the context

ISIS has subdivided its analytical platforms in two departments: (i) services for (physical) chemists, which includes three NMR instruments, four mass spectrometers, three FT-IR, Fluorimeter, and Raman instruments, and microscopic facilities; (ii) Nanofabrication facilities, e.g. XPS, clean room, FIB, and mask aligner. All equipment is accessible for staff and students after a specific training by the responsible technician. With the extension of ISIS, several new platforms have been installed. Furthermore, the University of Strasbourg together with CNRS and Inserm has set up a broader network of service platforms called CORTECS. It is expected that the ISIS platform will be integrated with CORTECS in 2022, which is a good idea. Altogether, the committee feels that ISIS is attractive for scientists because of its excellent analytical platforms and the available technical facilities.

Weaknesses and risks linked to the context

The above-mentioned analytical and technical facilities are absolutely needed to carry out modern scientific research. ISIS has 18 permanent technical and administrative staff, of which only six are dedicated to science. Compared to the number of researchers at ISIS this is a very low number. Hence, long-term knowledge transfer and maintenance of instrumentation is not secured. With the expansion of the institute to ISIS-2 and CESQ this has become even more critical. As was already mentioned in the previous sections, this problematic issue should be discussed as soon as possible with the University of Strasbourg.

EVALUATION AREA 3: SCIENTIFIC PRODUCTION

Assessment on the scientific production of the unit

The scientific production of papers of ISIS is outstanding and the number of citations exceeds that of international standards. The quality of the work is extremely high and nearly all papers are published in top-tier journals. The quantitative publication record varies from group to group, which is related to the size of the group, but the quality of the papers remains constantly high even if the group is small. All scientific researchers, i.e. PIs, Ph.D. student and postdocs contribute to the writing of a paper. The scientific results produced at ISIS follow the principles of research integrity and open science. Altogether, the committee is very positive about the scientific production of ISIS.

1/ The scientific production of the team meets quality criteria.

Strengths and possibilities linked to the context

The scientific production of the teams of ISIS is very high and amounted to 530 papers in the past period. The number of citations since 2016 exceeds 68,000 and hence the average publication citation rate is much larger than 100, which is very high compared to international standards. Not only the quantity of papers by ISIS meets the quality criteria, but also the quality of the papers. Nearly all of them were published in top journals such as *Nature*, *Science*, *the Nature family of journals*, *the Journal of the American Chemical Society*, *Angewandte Chemie*, and *Physical Review Letters*. The papers of the team leaders submitted in the self-assessment portfolio clearly reflect this high quality. The excellence of research at ISIS is also reflected in the prizes and awards the team leaders have received in the past period, and in the memberships of learned societies and honoris causa doctorates.

Weaknesses and risks linked to the context

The quantity of papers produced by researchers at ISIS is very high and the quality of the work is excellent. The committee sees no weak points.

2/ Scientific production is proportionate to the research potential of the unit and shared out between its personnel.

Strengths and possibilities linked to the context

The number of papers produced by the groups at ISIS is very high, but there are variations in the scientific production between the various groups. This is proportionate to the research potential of the individual research units. More research grants allow a PI to hire more Ph.D. students and postdocs and this undoubtedly increases the output. According to the self-assessment document all personnel, i.e. PI, Ph.D. students, and postdocs are involved in the writing of the papers, which is good.

Weaknesses and risks linked to the context

As mentioned above, the overall production of articles at ISIS is high, although there are variations between the individual units, which are related to the group size and the extent to which funding is acquired. This is not a real risk, although it is advisable to keep an eye on this fundraising issue for a single individual group. If the number of funds falls below an acceptable level, action should be taken.

3/ The scientific production of the unit complies with the principles of research integrity, ethics and open science.

Strengths and possibilities linked to the context

ISIS has produced an internal document in which the policy of the institute regarding the monitoring and protection of scientific results is outlined. This obligates the research staff to keep a laboratory notebook with clear, concise, and chronological entries, which guarantees the traceability of the data and the transmission of

the results. This is also a legal requirement if results are going to be patented later. The laboratory notebooks are kept in the laboratory, even after departure of the researcher. Scientific articles are published open access and deposited in the univOAK institutional archive of the University of Strasbourg. Students are trained in ethics and open access policies. All measures taken by the institute are in line with the principles of research integrity and open science, which is rewarding.

Weaknesses and risks linked to the context

There are no weaknesses and risks related to research integrity and open science. All necessary measures have been taken by the institute.

EVALUATION AREA 4: CONTRIBUTION OF RESEARCH ACTIVITIES TO SOCIETY

Assessment on the inclusion of the unit's research in society

The presence of industrial departments in ISIS is a very efficient way of transferring the results of academic scientific research to industry and has resulted in many patents and three spin-off companies. In this regard, the institute is an example for other institutes in France and Europe, and the committee recommends continuing the same path. ISIS is very active in bringing its research activities to society. This occurs through the large number of seminars that are held annually, the organization of scientific meetings that are connected to artistic or cultural events, the activities in which ISIS is placed in the spotlight (e.g. the visit of the Dalai Lama, and the celebration of the 10th anniversary of the European Research Council). Exposure of ISIS also occurs very efficiently thanks to the modern social media, e.g. Facebook, Twitter, and YouTube. The committee did not see weaknesses or risks for the future and recommends the institute to continue its successful path of communication with society.

1/ The unit stands out by the quality of its non-academic interactions.

Strengths and possibilities linked to the context

Already from its start the policy of ISIS was to host industrial departments. In the past period this involved six industrial partners, i.e. BASF, Strem, Syndivia, CardioRenal, Qfluidics, and odimma. This organizational set-up is excellent, as it facilitates the transfer of knowledge to industry. The impact of the endeavors of ISIS is evident from the filed patents (8 patents and invention disclosures since 2016), the creation of spin-offs (3 from ISIS PIs) and the fact that the team leaders frequently act as consultants for industry. Several PIs developed maturation projects with industrial partners, e.g. Prof. Thomas Hermans and Prof. Luisa De Cola. This has resulted in two start-up, i.e. SiBreaX, which develops new therapeutic agents, and Qfluidics, which creates a magnetostaltic pump based on ferrofluidic liquid tubes. For many years ISIS has been involved in disseminating its output and achievements with society. The institute organized many events and participated in major exhibitions, institutional ceremonies, and cultural events, which is nice. Since 2016 as many as 93 monthly seminars were organized, including 36 Young Scientists seminars and 57 "Conferences de ISIS", which are plenary lectures by top researchers. Due to the corona crisis a number of these seminars were given by video. It is very nice that ISIS organizes every year so-called "les Rencontres de ISIS" meetings in which science is brought closer to society. The chosen topics are of wide interest and include chemistry and chocolate, chemistry and food, etc. These meetings are usually connected to an artistic or cultural event in Strasbourg. The awarding of a prize to an ISIS PI is often used to put the institute in the spotlight, e.g. via interviews, short movies, or photo exhibitions, which is excellent. Visits of representatives of the government or of European institutions to ISIS, e.g. as in March 2017 when the 10th anniversary of the European Research Council was celebrated, also are instrumental in bringing science and technology to society. Announcements of important events and major scientific results are disclosed via the ISIS website and the PR canals of the University of Strasbourg, but also via social media such as Twitter and Facebook. The committee concludes that ISIS possesses a well-developed strategy for linking their scientific activities to the needs of industry and society. The presence of the above-mentioned industrial departments at ISIS is instrumental in this and makes that the different steps in the innovation process can be easily taken by the PIs at ISIS. It also helps match the expectations of the industry with those of the PIs, who can more easily decide whether a scientific finding is technologically mature enough for application, e.g. a patent or the start of a spin-off company. The committee, furthermore, concludes that ISIS' policy to share scientific results with society is very good.

Weaknesses and risks linked to the context

The committee notes that ISIS and its PIs are active in bringing their research to industry, e.g. via the presence of the industrial departments at ISIS, by filing many patents, and by starting spin-off companies. There is a useful underlying strategy, which is unique for France. Also, the interactions with society are very good. According to the committee there are no weaknesses or risks for the future. For reasons of efficiency the institute might consider assigning a person to coordinate the interactions with society. For the contacts with industry this not needed, as it is better that these take place directly between a PI and an industrial company.

2/ The unit develops products for the socio-economic world.

Strengths and possibilities linked to the context

The activities of ISIS aimed at bringing the results of its scientific activities to the economic world has already been mentioned above. In this context it is extremely efficient to have departments of different European companies in its building. A better interaction between science and industry is not possible and has already resulted in many new patents and the start-up of spin-off companies. Many PIs are also consultants for industry, which further strengthens the interaction with industry. The maturation projects of Profs. De Cola and Hermans have already been mentioned in section 1 above and these also evidence that the institute is very active in making links with the socio-economic world. Altogether, the committee feels that ISIS is doing extremely well regarding the aspect of developing products for the socio-economic world.

Weaknesses and risks linked to the context

The committee did not see any weaknesses or risks in the activities of ISIS to develop products for the socio-economic world and recommends the institute to continue the same path.

3/ The unit shares its knowledge with the general public and takes part in debates in society.

Strengths and possibilities linked to the context

ISIS is very active in sharing its knowledge with the general public, e.g. through meetings linked to cultural events, through press releases if a PI receives an award, and through newspapers, tv, and social media if an important discovery is made. As an example, Prof. John Moran has made nine YouTube videos to present his research and participated in 15 radio or TV programs, which is excellent. Other activities include the EUR "Complex Systems Chemistry", which is a new international integrated MSc/Ph.D. program carried out by Profs. Moran and Lehn and the Qustec project led by the EUCOR-European Campus, coordinated by Prof. Pupillo, which provide contributions to the societal impacts of training. In 2021, ISIS, the University of Strasbourg, and the CNRS have launched a project named aQCess aimed at building a quantum computer, which can perform calculations that are not possible with even the biggest supercomputers. This genuinely public facility will be a tool for research, multi-disciplinary teaching, and possible investment of companies. The activities of ISIS with respect to sharing knowledge with society is furthermore demonstrated by the organization and co-organization of nine events with the Presidency of the University of Strasbourg, the CNRS, Fondations de Strasbourg, Eurometropole de Strasbourg, and the region Grand-Est. These activities included amongst others the visit of the Dalai Lama to ISIS with round-table discussions on science, commitment to society and meditation, and the visits of the Minister of Research in 2018 and 2020. In 2016, ISIS hosted the awards ceremony for the project "Solutions d'Économie Verte en Entreprise", which was co-organized with the Eurometropole of Strasbourg and the University of Strasbourg. It is worth mentioning that in February 2017 a coffee-theater play "Everybody is going down", in which staff of ISIS and the University of Strasbourg and the external public are brought together, took place at ISIS. The institute also participated in several other events, e.g. the Women in Science action of IUPAC in 2020 and the European Disability day in 2021. All this shows that ISIS is doing extremely well regarding the aspects of sharing knowledge with the general public and communicating with society.

Weaknesses and risks linked to the context

The committee does not see any weaknesses or risks for the future.

C – RECOMMENDATIONS TO THE UNIT

Recommendations regarding the Evaluation Area 1: Profile, Resources and Organisation of the Unit

1. It is recommended to reconsider the science policy of ISIS and to strengthen the chemistry-biology interface of the research at the institute. The latter should preferably be achieved by hiring a high-profile senior scientist with a background at the interface of chemistry and the life sciences.
2. The committee notes that the administrative support staff of ISIS is minimal. This also holds for the technical staff with is too low to support all groups. With the expansion of ISIS with ISIS-2, which has been accompanied by a considerable increase in surface area, this problem has become even worse and is a threat for safe working in the building. The committee recommends taking immediate action.
3. The policy of ISIS is to keep junior staff for only 6 years after which they must move elsewhere. By itself, this is a good course of action, because it preserves momentum. On the other hand, the rules should not be so strict that it becomes impossible to keep a junior staff member if he or she performs outstandingly.
4. The committee notes that in the past period quite some very talented senior and junior staff members have left ISIS and another one has announced that he will leave next year. This high turnover of staff may be a threat for the future because it may disrupt the age balance within ISIS. According to the committee this balance is currently fragile. It is recommended to investigate in detail what steps must be taken to deal with this problem.
5. The current director will now step down and a new one must be found. Given the complexity of the director functions a high-profile person with an excellent scientific background and good social and managerial skills is needed. This is not easy, and the committee hopes that the institute will be able to find such a person at short notice.

Recommendations regarding the Evaluation Area 2: Attractiveness

1. The gender balance of young scientist at ISIS is 106 men and 53 women, which is acceptable. Unfortunately, there is no female senior PI and only one female junior PI. This unbalance is a strong weakness and a risk for the future, as it may decrease the attractiveness of the institute. The committee strongly recommends hiring more talented female senior and junior PIs in the coming years. In this connection one may consider creating a special chair and a special prize for female scientists, which is financed by industry (L'Oréal?) or by a philanthrope. This will put the spotlight on ISIS as a center for talented women.
2. ISIS is underfunded by the French authorities and most of the funding comes from outside France, e.g. the European Community. This issue should be analyzed further and discussed with the University of Strasbourg and the CNRS to make the financial future more sustainable. The hiring of more technical support staff is recommended. In order to be eligible for funding of support staff by the CNRS and the University of Strasbourg several instruments should be brought together to form a new platform.

Recommendations regarding Evaluation Area 3: Scientific Production

The scientific production of papers and patents is remarkably high, and the quality extremely high, as follows amongst others from the high number of citations, which exceed that of international standards. The committee recommends continuing along the same path in the future. It was noticed that the number of published papers varies from group to group. This fact must be related to the number of Ph.D. students and postdocs in a group. It may be worthwhile that senior PIs coach young PIs to help them improve their publication record, if needed.

Recommendations regarding Evaluation Area 4: Contribution of Research Activities to Society

The presence of industrial departments at ISIS is an excellent way to transfer scientific knowledge to industry and has resulted in many patents and three spin-offs. The committee recommends continuing this successful format. ISIS is very active in bringing the results of its scientific activities to society and uses various ways to do this. No improvements on this activity are needed.

TEAM-BY-TEAM ASSESSMENT

Team 1: Laboratory of Supramolecular Chemistry
 Name of the supervisor: Prof. Jean-Marie Lehn

THEMES OF THE TEAM

This group works on many areas, whose common denominator is supramolecular chemistry with applications in the field of energy and electron transfer processes in cryptates, the design of macrocyclic complexing agents, supramolecular catalysis, supramolecular materials, bioorganic chemistry, and more recently constitutional dynamic chemistry. The group has constructed complex higher order constitutional dynamic networks containing multiple constituents derived from hydrazone, acylhydrazone, and imine ligands, displaying adaptive behavior in response to effectors, e.g. metal ions. Characteristic features of these systems are multiple agonistic and anti-agonistic regulation, agonist amplification, and synergistic operation. They can be used for information storage and as complex supramolecular materials.

CONSIDERATION OF THE RECOMMENDATIONS OF THE PREVIOUS REPORT

The previous evaluation was extremely positive and stated that Prof. Lehn was the undisputed leader in its field, who continued to produce over 15 papers per year in top journals, which are receiving circa 3,000 citations per year. Given the undiminished dynamic behavior and productivity of the team leader, no weaknesses were identified. The research group and its team leader were strongly encouraged to continue their research activities at the same level. The committee concludes that this high level was maintained in the past evaluation period. The provided papers show that the group is still doing cutting-edge research, which is receiving international attention.

WORKFORCE OF THE TEAM

Permanent personnel in active employment	
Professors and associate professors	0
Lecturer and associate lecturer	0
Senior scientist (Directeur de recherche, DR) and associate	0
Scientist (Chargé de recherche, CR) and associate	1
Other scientists (Chercheurs des EPIC et autres organismes, fondations ou entreprises privées)	0
Research supporting personnel (PAR)	2
Subtotal permanent personnel in active employment	3
Non-permanent teacher-researchers, researchers and associates	2
Non-permanent research supporting personnel (PAR)	2
Post-docs	2
PhD Students	3
Subtotal non-permanent personnel	9
Total	12

EVALUATION

Overall assessment of the team

Prof. Lehn is the founding father of the field of supramolecular chemistry. He continues to make new contributions and to develop new directions, which are inspiring for other researchers, particularly young starting scientists. His current work on constitutional dynamic chemical systems is very elegant and opens many possibilities for further research. Although Prof. Lehn's studies are fundamental in nature, he has an open eye for applications, as is shown by his strong past track record. In conclusion, the group is doing extremely well and is expected to maintain a high visibility in the field.

Strengths and possibilities linked to the context

Attractiveness

This is a small but excellent group working on original and promising topics with a remarkable synergy between fundamental and applied science. The field of research of Prof. Lehn is modern and inspiring for many other research fields. The word "Supramolecular" is not linked exclusively to chemistry anymore, but nowadays also to the fields of (molecular) biology and even medicine. Especially the younger generation of scientists has benefited from the scientific endeavors of Prof. Lehn. He has trained many Ph.D. students (9 including 3 in progress), postdocs (15) and other researchers (8) in his group and these have now academic positions at institutes and universities all over the world. The research activities of the group have been disseminated through conferences and lectures (242) by the PI all over the world. The attractiveness of the group remains very high, as evidenced by the fact that it welcomed three visiting researchers in the reference period, an attractiveness that certainly will continue to exist in the future. This attractiveness is also the result of the group leader's dynamic attitude, which has resulted in new European (1 ERC Advanced grant, 1 ITN Marie Curie network) and National (2 ANR, 2 PIA) funding since 2016. This once again reflects the team's very good reputation at the national and international levels.

Production

This small group has been extremely productive with 54 publications over the reference period in top journals (*Nature Communications*, *JACS*, *Angewandte Chemie*, *Chemical Science*), covering different topics related to supramolecular chemistry. The studies of the group are very solid, both theoretically and experimentally, and are based on original ideas of the team leader. They have contributed significantly to the increase of knowledge. The scientific production of the group is in line with its size and all researchers (Ph.D. students, except one, postdocs, and other contractual researchers) contributed to the output. The group prefers quality of publications over quantity, which is to be valued.

Inclusion in society

The group is very much aware of the fact that science can help solve issues related to society. In that sense it aims at using fundamental knowledge to solve problems related to materials, catalysts, and medicine. The supramolecular materials, which were for the first time reported by the team leader in a paper in the Proceedings of the National Academy of Science in 1990, are a good example of this. They mimic the combined covalent and non-covalent materials found in nature and the idea has been emulated by many groups all over the world. It has resulted, among other things, in the development of a supramolecular biomaterial by an independent biotech company, which since 2013 is in use in the clinic in pediatric vascular surgery. The team leader has also developed an anti-cancer drug, which is now in clinical trial in patients. Cooperation with companies is high on the agenda of the team leader, and every time a research activity has a positive outcome, contact is made with a company. The team leader has been co-founder of several start-up companies and one more is in the process of being set up. The group is active in making the results of their scientific work available to society, e.g. through free general public lectures, of which many were presented by the team leader for high school students, universities, science museums, etc.

Weaknesses and risks linked to the context

Attractiveness

The group is still at the forefront of science in the field of supramolecular chemistry and has not shown any signs of decline. The team leader is still energetic and full of new ideas. He is the figurehead of the institute and the

committee is confident that he will continue to be the visible leader of supramolecular chemistry in France and in the world.

Production

In the period of assessment, the group has published many papers with cutting edge science in top journals. There is no sign of decline in the quality and quantity of the papers. The team leader continues to train Ph.D. students and postdocs and hopes to do so in the near future as well. There are no weaknesses or risks, apart from the inevitable risk of the advancing age of the team leader, as already mentioned.

Inclusion in society

The team leader is very active in bringing the results of his scientific studies to society and the general public. However, no industrial contacts or valorization projects with associated patents is mentioned during the reference period, even if it is obvious that the innovative and very fruitful knowledge transfer counteracts this finding. The corona issues have halted this process of knowledge transfer, but the team leader is eager to get it started again. The committee hopes that he will be able to travel again and give lectures at institutes and universities all over the world. The committee sees no weaknesses here.

RECOMMENDATIONS TO THE TEAM

The research team is still leading in the field of supramolecular chemistry and its current extensions in the direction of complex matter. The research program is ambitious, as it should be, and the committee recommends the team leader to continue his path. A wealth of new results is expected in the near future and this will be of great significance to chemistry as a whole. In the coming years the team leader should receive all possible support for his program.

Team 2: Laboratory of Quantum Physics
 Name of the supervisor: Mr Guido Pupillo

THEMES OF THE TEAM

The team is internationally recognized for the numerical studies of strongly correlated quantum matter. Thanks to an interdisciplinary approach, they have been working on a wide range of problems ranging from condensed matter to atomic and molecular physics and identified relevant applications to quantum information and simulations. The group counts on several collaborations with leading scientists worldwide. At ISIS it has established a very productive collaboration with the groups of Prof. Thomas Ebbesen and Prof. Shannon Whitlock. Moreover, together with Prof. Whitlock, it is working on establishing the first open access quantum computing platform in France.

CONSIDERATION OF THE RECOMMENDATIONS OF THE PREVIOUS REPORT

The previous evaluation was very positive. In the meantime, the group has started a series of new activities in many directions, of which the outcome remarkably surpasses the expectations of the previous report.

WORKFORCE OF THE TEAM

Permanent personnel in active employment	
Professors and associate professors	1
Lecturer and associate lecturer	0
Senior scientist (Directeur de recherche, DR) and associate	0
Scientist (Chargé de recherche, CR) and associate	1
Other scientists (Chercheurs des EPIC et autres organismes, fondations ou entreprises privées)	0
Research supporting personnel (PAR)	1
Subtotal permanent personnel in active employment	3
Non-permanent teacher-researchers, researchers and associates	0
Non-permanent research supporting personnel (PAR)	1
Post-docs	2
PhD Students	7
Subtotal non-permanent personnel	10
Total	13

EVALUATION

Overall assessment of the team

The Team of Quantum Physics is one of the world leaders in the numerical studies of quantum many-body systems. Its contributions are of outstanding quality and are highly original. The team is synergetic and at the same time an important pillar for the research in the quantum realm, ranging from few to many-body systems. The group impressively manages to keep an outstanding research profile and at the same time it develops a scientific, didactic, and technological infrastructure that contributes to the profiling of Strasbourg as an emerging center of excellence for quantum technologies.

Strengths and possibilities linked to the context

Attractiveness

The field of research of the team completes and extends the research activities at ISIS. It matches the institute objectives and has boosted its impact by providing visibility in the quantum optics, many-body physics, and quantum information communities. The team attracts talented graduate students and postdocs, who perform excellent research work under the PI's and his collaborators' supervision. The acquired funding over the latest years is impressive, and further confirms the scientific reputation and excellence of the team. The research activities have been disseminated through conferences and lectures by the PI and his close collaborators all over the world, and by activities on social media. The attractiveness of the team is very high. It has organized a prominent international forum, with more than 500 participants and 30 world leading companies.

Production

Over the years the team has published a good number of high impact papers on different topics, ranging from quantum information, strongly-correlated quantum matter, and molecular physics. The studies of the team are very solid, insightful, and original, the journals in which the results are published are of high impact. The scientific production of the team is in line with its size. The committee appreciates that the team prefers quality of publications over quantity.

Inclusion in society

The team is very active in the dissemination and transfer of knowledge outside the academic environment. In addition to divulgation activities, the committee highly values the projects with industrial partners (BASF and IBM), including the training networks (MOQS and QUSTEC), which programmatically include internships of PhD students in industry and, vice versa, academic training for young researches working in companies. The committee notes that Prof. Pupillo himself coordinates the ITN network MOQS and is the scientific director of QUSTEC. It is especially worthwhile to mention the project aQCess on establishing a quantum computing platform in France. This is an extraordinary service to the scientific community and to society, which the committee highly appreciates. Several valorization projects are in progress with the objective of creating start-ups.

Weaknesses and risks linked to the context

Attractiveness

The committee does not identify any weakness or risks for the future.

Production

The production of the team is appreciable, both with respect to quality and quantity of the papers. The committee does not identify any weakness or risks for the future.

Inclusion in society

The involvement of ISIS, and especially of this team and the team of Prof. Whitlock, in the long-term perspective of the aQCess project is not clear to the committee.

RECOMMENDATIONS TO THE TEAM

The research team performs excellent research in theoretical quantum physics, it is successful in terms of scientific production, attractiveness, and funding. Moreover, the team is very active and successful in developing and establishing research and technological infrastructures. In the coming years the team leader should receive all possible support for his program.

Team 3: Laboratory of Nanostructures
 Name of the supervisor: Mr Thomas Ebbesen

THEMES OF THE TEAM

The team has pioneered the field of nano-optics and plasmonics, to which it continues to actively contribute. It is currently world-leading in this field. Its expertise is to combine chemical and molecular physics with quantum optics. The team is well established and is very productive. More recently, it has focused its activities on quantum electrodynamics with organic molecules, analyzing several novel and promising possibilities, such as the control of chemical reactions and the interactions of molecules with chiral light.

CONSIDERATION OF THE RECOMMENDATIONS OF THE PREVIOUS REPORT

The previous evaluation of the team was excellent with respect to all the different criteria that were considered. The evaluation report highlighted the pioneering scientific studies in the fields of plasmonics, light-matter interactions, and chirality, and praised the outstanding production of the team (66 publications in top-tier journals). The high impact of the research activities of the team and its international recognition were also noticed.

WORKFORCE OF THE TEAM

Permanent personnel in active employment	
Professors and associate professors	1
Lecturer and associate lecturer	0
Senior scientist (Directeur de recherche, DR) and associate	1
Scientist (Chargé de recherche, CR) and associate	1
Other scientists (Chercheurs des EPIC et autres organismes, fondations ou entreprises privées)	0
Research supporting personnel (PAR)	1
Subtotal permanent personnel in active employment	4
Non-permanent teacher-researchers, researchers and associates	0
Non-permanent research supporting personnel (PAR)	0
Post-docs	6
PhD Students	6
Subtotal non-permanent personnel	12
Total	16

EVALUATION

Overall assessment of the team

The team is world leading in the field of nano-optics and continues to make new exciting contributions. It constantly takes new directions, which are inspiring for other researchers, particularly young scientists. The current research activity of the team on the control of chemical processes using vibrationally strongly coupled systems is ground-breaking and opens promising avenues for fundamental research at the interface between quantum optics and molecular physics. In conclusion, the team is doing extremely well and is expected to maintain a high visibility in the field.

Strengths and possibilities linked to the context

Attractiveness

During the evaluation period, the team continued to develop innovating research directions, often in collaboration with teams inside and outside ISIS. In this connection it is worth mentioning the new theme "Polaritonic chemistry", which is highly valued. The projects of the team are cutting-edge, very visible and highly recognized. The results of its studies are published in the best international journals, leading to an outstanding scientific recognition. The committee emphasizes that the team leader received an ERC advanced grant (his second one) during the evaluation period and was awarded several prestigious awards and distinctions, e.g. the Grand Prize of the "Maison de la Chimie" Foundation, the CNRS gold medal, and the National Order "Légion d'Honneur". All these endeavors make that the group is very attractive for PhD students and post-docs. They have the security of being able to participate in excellent projects, which will lead to high level papers. Furthermore, they will receive an excellent training, allowing them to successfully pursue an academic career or a career in industry. The team has given numerous lectures and presentations in international workshops, which further adds to its attractiveness.

Production

With more than 36 papers in the highest impact factors journals, the scientific performance of the team during the period of assessment is excellent, not only with respect to the numbers of papers, but also with respect to their quality. They were published in top journals, such as *Science*, *Science Advances*, *Nature Nanotechnology*, *JACS*, *Angew. Chem.*, *Nano Letters*, *ACS Nano*, and *Phys. Rev. Lett.* It is worth noting that several of these papers already received several hundreds of citations, which witnesses the high visibility of the research performed. Furthermore, the spectrum of the journals where the papers are published illustrates that the work of the group is highly interdisciplinary.

Inclusion in society

The group is very much focused on the fundamental aspects of its research and is well aware of this. The team leader discusses with industrial partners the potential applications of the group research. The team also files patents regularly. The results of their work are presented to the general public through interviews with journalists and publications in journals with a broader general audience to reach industrial actors.

Weaknesses and risks linked to the context

Attractiveness

The team is leading worldwide and does not show any sign of weakness.

Production

The results of the scientific studies are published in the best journals. No weakness has been identified.

Inclusion in society

The research of the group is fundamental in nature, and this makes that it is not always easy to establish partnerships with groups in society. Nevertheless, the team leader is making all efforts to find industries interested in the development of new technologies based on his research activities.

RECOMMENDATIONS TO THE TEAM

No changes are required in the policy and research direction of the team. The committee recommends the group to continue its very successful scientific path of developing new forefront projects at the interface of physics and chemistry. The team leader must keep up the pressure on industrial partners, stimulating them to invest in R&D based on the projects of the team.

Team 4: Laboratory of supramolecular biomaterials and chemistry
 Name of the supervisor: Ms Luisa De Cola

THEMES OF THE TEAM

During the evaluation period, four research areas have been addressed by the team, i.e. the synthesis and the physical studies of: (i) electroluminescent materials; (ii) supramolecular self-assemblies; (iii) porous materials; and (iv) hybrid materials for in-vitro and in-vivo imaging. These research themes involve multidisciplinary approaches and address hot topics at the forefront of chemistry and at the interface with physics for the luminescence applications, and at the interface with biology/medicine for the drug delivery part in cancer research.

CONSIDERATION OF THE RECOMMENDATIONS OF THE PREVIOUS REPORT

The previous evaluation was extremely positive, and the team and its leader were strongly encouraged to continue their research activities at the same level. The committee recommended reinforcing the PI's team and strengthening the link with the industry. These recommendations have been addressed: the team was reinforced by the hiring of Dr. Alessandro Aliprandi, who joined the team as a CNRS engineer, allowing it to further develop its top research activities and attract more students. Also, the interactions with industry were strengthened. Important discoveries have been patented (8 in the period 2016/20), which resulted in a substantial increase in industrial collaborations: with Roche Diagnostics on the development of electro-chemiluminescent labels, with L'Oréal on the realization of materials that are able to entrap active species and be degraded under light exposure, with Syngenta on the destruction of specific insects, with Takeda on the encapsulation and delivery on demand of proteins, and with QVentis on the development of hyaluronic acid based hydrogels for cosmetic applications.

WORKFORCE OF THE TEAM

Permanent personnel in active employment	
Professors and associate professors	0
Lecturer and associate lecturer	0
Senior scientist (Directeur de recherche, DR) and associate	0
Scientist (Chargé de recherche, CR) and associate	0
Other scientists (Chercheurs des EPIC et autres organismes, fondations ou entreprises privées)	0
Research supporting personnel (PAR)	0
Subtotal permanent personnel in active employment	0
Non-permanent teacher-researchers, researchers and associates	0
Non-permanent research supporting personnel (PAR)	0
Post-docs	0
PhD Students	1
Subtotal non-permanent personnel	1
Total	1

EVALUATION

Overall assessment of the team

The team studies the interaction of light with (self-assembled) molecular matter and is taking a leading position in this field. PI has a great visibility and her research group is recognized as being of high international level, as evidenced by the high number of high-impact publications and patents. The overall assessment of the team is excellent in all aspects.

Strengths and possibilities linked to the context

Attractiveness

The scientific themes of the team have in common the study of the interaction of light with molecular matter and the reactivity that is associated with this interaction. For this, the team is renowned nationally and internationally. Research is conducted primarily at the fundamental level, but the team also responds to important socio-economic issues and the team has strengthened its thematic links with the industrial world during the evaluation period. More precisely, the originality of the work not only lies in the advancement of science but also in possible applications for society. For example, the work on self-assembly has generated a new type of sensors and the work on injectable hydrogels has been explored in different hospitals for the treatment of fistulas and other pathologies. Also, the strong collaborations with IRCAD and IHU have been extremely important for the translation of some of the materials developed by the team to clinical applications. The team leader benefits from an international reputation which is reflected in a very large number of invitations to international scientific congresses (50). The AAP success rate in the four research themes developed by the team is very good. In addition, the recent evolution of the topics reflects the dynamics of the team and its desire to respond to major societal challenges.

Production

The activities of the team have led to a high number of top-quality papers (68 in the period 2016-2020) in highly ranked journals such as *Nature Chemistry*, *Nature Communications*, *JACS*, and *Angew. Chem.* This number is somewhat lower than in the previous period, but this is compensated by the larger number of patents. Eight patents have been deposited in the period of evaluation, which is the result of an increase of industrial collaborations: with Roche Diagnostics on the development of electro-chemiluminescent labels, with L'Oréal on the realization of materials that are able to entrap active species and be degraded under light exposure, with Syngenta on the destruction of specific insects, with Takeda for the encapsulation and delivery on demand of proteins, and with QVentis on the development of hyaluronic acid-based hydrogels for cosmetic applications.

Inclusion in society

Besides the fundamental science for the scientific community, the team has participated in science fairs, expositions, and school seminars (famous is Luisa De Cola's talk on chocolate). The research of the team has also received attention in newsletters and journals for the general public. Furthermore, the group participated in interviews and round table discussions on nanomedicine and nanomaterials. It is evident that the dissemination of scientific results to society has been one of the missions of the team.

Weaknesses and risks linked to the context

Attractiveness

The committee did not identify weaknesses or risks.

Production

The committee did not identify weaknesses or risks.

Inclusion in society

The committee did not identify weaknesses or risks.

RECOMMENDATIONS TO THE TEAM

The laboratory of Supramolecular Biomaterials and Chemistry of Professor Luisa De Cola and Dr. Alessandro Aliprandi is excellent at all levels. Unfortunately, Professor de Cola recently moved to the « Università degli Studi di Milano & Istituto Negri » and Dr. Aliprandi accepted a position elsewhere. The departure of this team raises the urgent question how ISIS will strengthen its research activities at the interface with biology and how it will cope with the low number of female PIs within ISIS.

Team 5: Laboratory of chemical catalysis

Name of the supervisor: Mr Joseph Moran

THEMES OF THE TEAM

The team led by Prof. Moran is active in three very different areas of research. First, this team works on prebiotic chemistry to understand the origin of life. It also works, in collaboration with another team within ISIS (Prof. T. Ebbesen), on the use of vibrational strong coupling to alter the rates and selectivity of chemical reactions. Finally, the team is active in the field of organic synthetic methodology.

CONSIDERATION OF THE RECOMMENDATIONS OF THE PREVIOUS REPORT

The previous evaluation was very positive. The committee especially valued the original studies of the team on self-organized reaction networks, with a focus on the understanding of the transition from chemistry to biochemistry. The committee also recommended to consider a broader perspective studying important catalytic systems of synthetic interest. The team has acted on this suggestion.

WORKFORCE OF THE TEAM

Permanent personnel in active employment	
Professors and associate professors	1
Lecturer and associate lecturer	0
Senior scientist (Directeur de recherche, DR) and associate	0
Scientist (Chargé de recherche, CR) and associate	1
Other scientists (Chercheurs des EPIC et autres organismes, fondations ou entreprises privées)	0
Research supporting personnel (PAR)	0
Subtotal permanent personnel in active employment	2
Non-permanent teacher-researchers, researchers and associates	1
Non-permanent research supporting personnel (PAR)	0
Post-docs	5
PhD Students	8
Subtotal non-permanent personnel	14
Total	16

EVALUATION

Overall assessment of the team

The investigations of the team in the field of prebiotic chemistry aimed at understanding the origins of life are excellent. They focus on the development of self-organized systems that occur without human intervention, which is unique. The team also pioneered, in collaboration with team 3 (Prof. T. Ebbesen), the use of vibrational strong coupling as a tool to alter the rates and selectivity of ground state chemical reactions, which has led to exciting results. Recently, the team has demonstrated how vibrational strong coupling can be used to change the stereoselectivity predicted by the Woodward–Hoffmann rules in the thermal electrocyclic ring opening of a cyclobutene derivative. The research of the team in organic synthesis is more diverse. In this area, one of the topics in which it has received international recognition, is the use of fluorinated alcohol solvents to perform selective transformations in organic synthesis.

Strengths and possibilities linked to the context

Attractiveness

The team has published results of significant interest in very different areas of research, including prebiotic chemistry, the use of strong vibrational coupling to alter chemical reactions, and the use of fluorinated alcohols to achieve selective chemical transformations in organic synthesis. Its research is cutting edge and has a high international visibility. The team leader is the recent recipient of the Liebig Lectureship of the German Chemical Society (2022) and he was selected as a Junior Member of the "Institut Universitaire de France". He also was awarded the prize "Forcheurs Jean-Marie Lehn 2020" (shared with Harun Tüysüz).

Production

The team has a strong track record of publishing top papers in high-ranking journals and favors quality over quantity. The overall production and the average quality of the articles are excellent considering the size of the team. In the past, the team leader already had received an ERC Starting Grant and he now got an ERC Consolidator Grant (2021-2026), which will further boost the scientific activities of the team.

Inclusion in society

The team, including the PI and several of his PhD students, have participated in many outreach activities. They have produced several YouTube videos and participated in programs on radio and on TV. The research of the team has been highlighted in *National Geographic*, *Chemical & Engineering News*, *La Recherche*, *Today's Science*, *New Scientist*, and *Science Magazine*. Together with Professor Lehn, Prof. Moran is responsible for the EUR "Complex Systems Chemistry" program, which is an international integrated MSc/PhD program. Although most of the research projects of the team are on fundamental science, projects of interest to industry, such as the catalytic dehydrative substitution of alcohols, are also addressed nicely. Prof. Moran also collaborates with several pharmaceutical companies.

Weaknesses and risks linked to the context

Attractiveness

The team has conducted conceptually innovative research in very diverse areas. Although this could lead to a lack of focus, the high diversification of research interests is not perceived as a significant weakness. There are no other points that can be viewed as weaknesses or risks for the future.

Production

The publication record in the period of assessment is very good. Given the fact that the team leader recently received an ERC Consolidator grant, the production of the team can be expected to increase further in the near future. No clear weaknesses or risks are perceived.

Inclusion in society

The team is very active in bringing its research to society, as is shown above. Also, the contacts with industry are very good and can be expected to grow further. There are no weaknesses or risks for the future.

RECOMMENDATIONS TO THE TEAM

Unfortunately, the committee was informed that Prof. Moran has decided to leave ISIS and to accept a position in Canada. This is a serious loss for the institute. The committee hopes that a new talented mid-career scientist can be hired soon to replace him.

Team 6: Laboratory of protein chemistry
 Name of the supervisor: Mr Vladimir Torbeev

THEMES OF THE TEAM

The team is active in the field of chemical and synthetic biology, working on four topics. The first one *Combinatorial chemical protein synthesis* is devoted to high-throughput combinatorial chemical protein synthesis developed as a new technology platform for chemical and synthetic biology. *Intrinsically disordered proteins* is the second project aimed at understanding the mechanisms of molecular recognition and complex formation involving intrinsically disordered proteins. The third topic *Protein misfolding and aggregation* is focused on the identification of molecular targets for designing new drugs against protein-misfolding diseases. The fourth project *Chemical physics of proteins* involves the modulation of enzyme activity by employing strong coupling of protein vibrations with the vacuum field using photonic cavities.

CONSIDERATION OF THE RECOMMENDATIONS OF THE PREVIOUS REPORT

The previous evaluation report commented that Prof. Torbeev is a very talented chemical biologist. His research was considered to be highly original and creative. The team is working on different topics and the previous report suggested that in the future, given the small size of the team, it might be better to focus on one or two projects that are the most successful ones. Prof. Torbeev may have complied with this suggestion, as he concentrated in the past period more on chemical protein synthesis as one of these preferred topics.

WORKFORCE OF THE TEAM

Permanent personnel in active employment	
Professors and associate professors	0
Lecturer and associate lecturer	0
Senior scientist (Directeur de recherche, DR) and associate	0
Scientist (Chargé de recherche, CR) and associate	0
Other scientists (Chercheurs des EPIC et autres organismes, fondations ou entreprises privées)	0
Research supporting personnel (PAR)	0
Subtotal permanent personnel in active employment	0
Non-permanent teacher-researchers, researchers and associates	0
Non-permanent research supporting personnel (PAR)	0
Post-docs	0
PhD Students	2
Subtotal non-permanent personnel	2
Total	2

EVALUATION

Overall assessment of the team

The team is leading worldwide in the development of new technologies to synthesize long and well-defined protein molecular constructs and is doing this with a high level of creativity and originality compared to the state of the art. The research of the group is fundamental, but with an open eye for applications, e.g. the development of drugs. Their studies on the modulation of enzyme activity through strong coupling of protein vibration modes is cutting-edge. The interactions with the socio-economic world are good. The size of the group is rather small, which may be a risk for the future.

Strengths and possibilities linked to the context

Attractiveness

The field of research of the team, i.e. protein chemistry, is highly relevant both from a fundamental point of view and in view of applications. Different projects are coordinated by the team leader, which are financially supported by Europe (ERC-Starting Grant) and national or local funding organizations (ATIP, FRC, CSC). The synthesis of long and well-defined protein molecular constructs is very difficult, and the group makes impressive progress in this direction by developing new technology platforms to realize this. They are among the few research teams in the world that can do this. The focus of the team on disordered proteins and proteins that contain disordered domains is excellent. Such proteins play important functional roles, e.g. in cellular signaling and regulation, and are not well understood. Furthermore, they are linked to diseases for which treatment is difficult. The studies of the team on the mechanism of protein misfolding and aggregation are also highly relevant as such misfolded structures are related to diseases like Alzheimer and Parkinson. Finally, the team tries to combine chemical biology with physics in their studies to modulate enzyme activity by coupling protein vibration modes with the vacuum field by means of photonic cavities (collaboration with Prof. Thomas Ebbesen). This is really cutting-edge research, which is only carried out at ISIS. The reputation of the team and more particularly of the PI is well known, notably through a remarkable number of invited lectures and seminars (20).

Production

The team is quite small and cannot be expected to produce an extensive series of papers. Given its size the productivity in the past period (14 papers) was good. More importantly, the group focuses on high quality work and this is reflected in the choice of journals, which include top journals such as *JACS*, *Angew. Chem.*, and *Chemical Science*, which is excellent. Further increase in production can be expected in the future, if the group increases in size. All group members, especially the PI and Ph.D. students contribute to the scientific production of the team (from 1 to 4 papers per Ph.D. student). Prof. Torbeev collaborates with top scientists from Strasbourg (e.g. Prof. Thomas Ebbesen and Prof. Bruno Kieffer) and elsewhere (e.g. Prof. William F. DeGrado from the University of California, San Francisco, Prof. Johanna Olesiak-Banska from WUST, Poland, and Prof. Stephen B. Kent from the University of Chicago).

Inclusion in society

The studies of the group on proteins are highly relevant for society and may lead to new drugs in the future. Prof. Torbeev collaborates with Inoviem Scientific on the development of artificial biomaterials for aorta prosthesis. A testing prototype has been developed and patented. In this connection a scientist from Inoviem worked for 8 months in his group in the framework of a SATT Conectus/CNRS/Unistra maturation project. A start-up company to bring this product to the market is considered for the near future. A start-up may also be possible for the work the team is doing on cancer-related intrinsically disordered proteins and tissue replacing biomaterials. The team is active in bringing its works to the general public; it organized an exhibition booth on the "Magic World of Proteins" at the "Fête de la Science" in Strasbourg in 2019. Further outreach activities involve a dedicated website and a YouTube video on their work.

Weaknesses and risks linked to the context

Attractiveness

As outlined above, the research of the team on the synthesis of long protein molecular constructs is highly relevant and there is no need to change the direction of this research, as it is successful. The committee noticed no weaknesses or risks.

Production

The team is small, and this inevitably influences the productivity. The committee hopes that the team leader will be able to raise additional money for his research activities, making that this aspect will be resolved in the future. On the other hand, the quality of the papers is excellent and there is no weakness regarding this aspect. The group has only one permanent member (the team leader) and lacks technical support staff. The latter is a weakness and a risk for the future as important knowledge may disappear when Ph.D. students and postdocs leave the group. Except for the very active team leader, the participation of contractual staff (Ph.D. and postdocs) in national and international conferences, workshops and seminars remains apparently low.

Inclusion in society

The team is doing its best to bring the results of their research to industry and society. This aspect may become a weakness and a risk if the team remains small and cannot give full attention to both fundamental research and applications. Also, the outreach activities, which are very good at this moment, may suffer from the small size of the team. Setting up further collaborations with other groups and companies may help resolve this issue.

RECOMMENDATIONS TO THE TEAM

The team is well on its way to become a leading group worldwide in the synthesis and applications of large proteins molecular constructs. The scientific ideas of the group leader are excellent and there is no need to change research direction. The team needs more sparring partners within ISIS on molecular biology aspects, but this may be compensated by setting up collaborations with groups working in the same field, either in Europe or oversea. Although very dynamic in the search for financial supports and coordination of several international, national and industrial projects, the small size of the team is a risk and all efforts should be taken to raise funding for further growth. It will thus be necessary to persevere in efforts to preserve certain competences, by attracting young researchers with the objective to consolidate the team's human resources. Furthermore, the committee recommends a more sustained contribution of all the members of the team, especially those receiving training, to congresses, seminars and conferences. Unfortunately, the team leader has left ISIS in 2021. The committee hopes that a new junior scientist with the same profile as Prof. Torbeev can be hired again soon.

Team 7: Laboratory of Nanochemistry
 Name of the supervisor: Mr Paolo Samori

THEMES OF THE TEAM

The team has demonstrated for several years that the approach of combining (supra)molecular science with 2D materials represents a powerful strategy to develop hybrid systems exhibiting a unique set of novel properties, which can be exploited to address important societal challenges in environmental and health monitoring, opto-electronics, digitalization, and energy-related technologies. During the evaluation period, the team worked on three main research themes: (i) chemistry of two-dimensional materials (graphene and other layered compounds), including the production, tuning of their properties, and fabrication of devices; (ii) multiscale tailoring of smart supramolecular systems, involving the development of multi-responsive coatings and composites; (iii) high-performance multifunctional materials and (nano)devices for optoelectronics, sensing applications, data storage, etc.

CONSIDERATION OF THE RECOMMENDATIONS OF THE PREVIOUS REPORT

The previous evaluation report commented that this research team, led by a scientist who is internationally highly visible and at the same time the director of ISIS, is in every respect exceptional, regarding the novelty of his research directions, his success in publishing high quality papers, and the education of young scientists. The committee recommended to continue this very positive and dynamic attitude in the next period of evaluation, which has been realized!

WORKFORCE OF THE TEAM

Permanent personnel in active employment	
Professors and associate professors	1
Lecturer and associate lecturer	1
Senior scientist (Directeur de recherche, DR) and associate	0
Scientist (Chargé de recherche, CR) and associate	0
Other scientists (Chercheurs des EPIC et autres organismes, fondations ou entreprises privées)	0
Research supporting personnel (PAR)	2
Subtotal permanent personnel in active employment	4
Non-permanent teacher-researchers, researchers and associates	3
Non-permanent research supporting personnel (PAR)	2
Post-docs	23
PhD Students	8
Subtotal non-permanent personnel	36
Total	40

EVALUATION

Overall assessment of the team

The team consists of highly creative researchers, which are very talented at converting innovative scientific problems into new high-risk/high-gain interdisciplinary research lines, thereby conveying and fertilizing interactions with scientists operating in different disciplines. The originality of this approach relies on combining sophisticated state-of-the-art nanotools (for fabrication and characterization) with supramolecular chemistry principles to develop structurally controlled functional nanomaterials and nanodevices, exhibiting special electronic, optical, and sensing capabilities. More precisely, the team has devised technological procedures and fabrication methods that have a strong impact on the development of new materials and on the realization and exploitation of "real-world" devices with prospects of high-performance applications for society and industry. The activities of the team is accompanied by an impressive publication track record and numerous international collaborations with industrial partners.

Strengths and possibilities linked to the context

Attractiveness

The team has demonstrated for several years that the combination of (supra)molecular sciences approaches with 2D materials represents a powerful strategy to develop hybrid systems exhibiting a unique set of novel properties, which can be exploited to address societal challenges in environmental and health monitoring, opto-electronics, digitalization, and related technologies. In particular, they evidenced that such a combination of materials offers the highest level of control over the bottom-up nanofabrication of functional hybrid materials, applicable in different research fields, for example: (i) liquid-phase exfoliation, which can be exploited to generate single-layer thick sheets of two-dimensional materials; (ii) formation of supramolecular hybrid architectures based on graphene oxide and organic multidentate ligands, exhibiting high affinity for metal ions and organic dyes offering applications in water treatment technologies; (iii) exploration of dynamic covalent chemistry approaches to form ultrasensitive hybrids that can be exploited as sensory materials for pressure monitoring; (iv) new examples of graphene-based composites as well as covalent organic frameworks and metal-organic frameworks and their hybrids. The latter are being successfully employed as active materials for energy storage. The recent results in these fields are very impressive and explain the fact that the funding for these ongoing projects (essentially European funding) is already secured for the next 5 years.

Production

The originality and quality of the work over the period of assessment is evidenced by 168 original scientific publications in high-impact journals (*Nature*, *Science*, *Nature Materials*, *Nature Nanotechnology*, *Nature Photonics*, *Materials Today*). In addition, this scientific production of the team includes many co-publications with partners of the highest international level (145 collaborative publications with one or more partners). Furthermore, we can cite 150 press releases and research highlights in various institutional and science news media (AlphaGalileo, C&EN, ChemistryViews, CNRS, CNRS Alsace, EurekAlert!, FRC, Graphene Flagship, ISIS, labex CSC, SCF, UNISTRA, etc.) and/or national newspapers (*Le Figaro*). The team established numerous international collaborations with industrial partners, such as STMicroelectronics (Italy), BASF (Germany), Nokia (United Kingdom), Metrohm DropSens (Spain), Aurel (Italy), APE Research (Italy), Graphenea (Spain), etc. in the framework of collaborative research projects, such as the Graphene Flagship (2013–2023), the MSCA Innovative Training Networks iSwitch (2015–2018) and ULTIMATE program (2019–2023).

Inclusion in society

The team encourages the hosting of professionals in its group and allows its personnel to stay at non-academic entities. Exposure of academic personnel to the private sector and vice versa is key towards intersectoral training and technology transfer. Hence, such an interchange is made a common practice in the endeavors of the team. The team has implemented a wide range of communication, dissemination, and public engagement activities aimed at broadening and promoting public awareness and understanding of science. These activities are not only tailored for scientists, but also designed to attract interest and participation of the wider society, thereby contributing to bringing science closer to the public.

Weaknesses and risks linked to the context

Attractiveness

The committee did not identify weaknesses or risks.

Production

The committee did not identify weaknesses or risks.

Inclusion in society

The committee did not identify weaknesses or risks.

RECOMMENDATIONS TO THE TEAM

The research developed in the team is highly original and creative. The status of the team leader is truly exceptional. The committee recommends the team leader to continue this successful path. The different staff members of the group are strongly connected to the different research topics making them key members of the research group. It will be important for some of them to secure their positions in the future.

Team 8: Laboratory of nonequilibrium complex systems
 Name of the supervisor: Mr Thomas Hermans

THEMES OF THE TEAM

In the self-description on its website, the Hermans group lists three activities: dissipative non-equilibrium self-assembly in supramolecular systems, chiral separation using Taylor-Couette flow, and microfluidics without walls. The core expertise in the Hermans group, as evidenced by prior production, is in the first of the three areas. They notably develop a supramolecular system whose assembly/disassembly cycles, size and internal order can be controlled using chemically fueled redox reactions. The latter two areas are newer to the team. The first one of these aims to reach molecular scale chiral resolution using shear flows and the second one is based on the use of ferrofluids under controlled magnetic field for fluidic applications. Prof. Hermans is also the Program Manager of a Joint European Disruptive Initiative (JEDI), the "billion molecules against Covid-19 GrandChallenge" that started in May 2020.

CONSIDERATION OF THE RECOMMENDATIONS OF THE PREVIOUS REPORT

Prof. Hermans has been Director of the Laboratory of non-equilibrium complex systems at ISIS in the period 2013-2019. In the previous report, the assessment of his scientific output, and future potential, was very positive, for many of the same reasons as indicated in the present report. Of note in the previous report are recommendations that Prof. Hermans make a visible break (in terms of independent publication) from his postdoctoral supervisor, which has been achieved satisfactorily in the present period.

WORKFORCE OF THE TEAM

Permanent personnel in active employment	
Professors and associate professors	0
Lecturer and associate lecturer	0
Senior scientist (Directeur de recherche, DR) and associate	0
Scientist (Chargé de recherche, CR) and associate	0
Other scientists (Chercheurs des EPIC et autres organismes, fondations ou entreprises privées)	0
Research supporting personnel (PAR)	0
Subtotal permanent personnel in active employment	0
Non-permanent teacher-researchers, researchers and associates	0
Non-permanent research supporting personnel (PAR)	0
Post-docs	0
PhD Students	10
Subtotal non-permanent personnel	10
Total	10

EVALUATION

Overall assessment of the team

The main theme of the team, non-equilibrium supramolecular assembly, is very timely, highly promising and a very challenging area of research, to which the team has made significant contributions. Results for the second and third areas are only just appearing, and their longer-term impact to the field is still open. We can, however, point out the creation of a startup Qfluidics founded in 2019 based on the liquid tube technology of the team. The Joint European Disruptive Initiative does not appear to fit into the picture well, being a project that seems relatively far removed from the other themes of the team. One may worry that this will distract the group from areas where it has otherwise unique strengths and positioning.

Strengths and possibilities linked to the context

Attractiveness

The work on non-equilibrium self-assembly is highly attractive in that it reveals the underlying principles for spatiotemporal construction of macroscopic order, or structures, from molecular components by self-assembly. Whereas much of the field remains wed to a relatively small number of molecular systems, e.g. BZ oscillators and related reaction-diffusion systems, Prof. Hermans has created novel instances, which assemble in ways not so far from what one observes in biological systems. The work is conceptually, and aesthetically, highly attractive. It is too early to say whether the chiral separation or microfluidic work rises to the top of their respective fields. The Joint European Disruptive Initiative project is driven by humanistic values and aims to fight against the Covid virus in a radical new collaborative approach to innovation. However, it is questionable whether this activity largely duplicates, and trails, work done in the pharmaceutical industry. The excellent attractiveness of the team can also be measured by its number of PhD (7) and postdocs (5) in 2022 and its success to obtain different grants notably ERC starting and Horizon 2020 grants. Prof. Hermans is also the coordinator of the Marie Skłodowska-Curie innovative training network "Creanet".

Production

The productivity of the team is not very high (13 papers in the reference period), although one should compare the output to that of other groups in the field. It may be a feature of the field as a whole. However, the publications appear in exceedingly high-profile journals (*Nature*, *Nature Comm.*, *Chem. Soc. Rev.*, *JACS*, etc.). The list of publications in the documentation provided for the evaluation ends in 2019, whereas the publication list on the Hermans group web page lists papers appearing in 2020 and 2021, probably reflecting his departure from ISIS in 2019. Prof. Hermans has received several awards, notably he was selected as young scientist for discussions in the World Economic Forum in 2019. The visibility of the team is good with 39 invited lectures since 2016.

Inclusion in society

One should be open-minded about "Inclusion in society" as a criterion. The supramolecular self-assembly work directly addresses a question of how nature build macroscopic objects from microscopic components, which is a fundamental question of great general interest. If one takes a narrow definition, then perhaps the involvement in the Joint European Disruptive Initiative makes a certain sense, but the committee is not convinced. A family of patents has been accepted during the period with some that are exploited by the Qfluidics start-up of which Prof. Hermans is the chief scientific officer, which is nice. He also participates to industrial partners committees. The team shares its knowledge with the general public through social networks, such as Youtube. Prof. Hermans is also involved in student training as the pedagogical director of a European master program.

Weaknesses and risks linked to the context

Attractiveness

One may worry that Prof. Hermans has over-diversified his group and will lose focus. The group leader is the only permanent researcher in the group up to now. Fortunately, a new assistant professor MCF will join the team in September 2022. The functioning of the team is essentially based on the success of calls for projects, mainly European, which maybe a risk for the future. One should consider that the previous report said, "The proposed topics require very broad knowledge in the team, which is only possible if an adequate number of researchers with different backgrounds are present. This would need a substantial funding to support such a highly

interdisciplinary group", which is still a valid statement. Addition of non-core themes to the group can therefore become detrimental.

Production

Similarly, an over-diversification into peripheral fields will certainly impact the output negatively in areas where Prof. Hermans is presently leading. This is a weakness and may be a risk for the future.

Inclusion in society

See comment above. The committee has some doubts whether the Joint European Disruptive Initiative project, although of value for society, fits well enough in the program of the team. It may duplicate work already done in industry.

RECOMMENDATIONS TO THE TEAM

The team has established leadership in non-equilibrium supramolecular assembly, which is a promising, high-profile field. The committee is not convinced that the team should invest time and energy in competing with the private sector in the fight against the Covid virus. The team leader, however, felt that this must be seen as a responsibility of scientists towards society.

Team 9: Laboratory of complex systems in synthesis and catalysis
 Name of the supervisor: Mr Pawel Dydio

THEMES OF THE TEAM

The junior group led by Prof. Pawel Dydio concentrates on complex catalytic cycles with a mechanistic focus, specifically treating multi-catalysis with cooperative reactions. The latter specialty is at the forefront of catalysis research, as it extends the network of reactions from a single catalytic cycle to multiple interacting catalytic cycles, with a concomitant increase in complexity. This complexity, however, offers the potential for novel transformations that otherwise are not possible, and it mimics the strategies in biological systems, i.e. biosynthesis with multienzyme complexes. The approach of the team is based on a combination of state-of-the-art computational and analytical studies. They already obtained significant results in the functionalization of strong C(sp³)-H, selective C-H borylation, and hydroformylation processes.

CONSIDERATION OF THE RECOMMENDATIONS OF THE PREVIOUS REPORT

Not applicable. Prof. Dydio started as a junior group leader in 2016.

WORKFORCE OF THE TEAM

Permanent personnel in active employment	
Professors and associate professors	0
Lecturer and associate lecturer	0
Senior scientist (Directeur de recherche, DR) and associate	0
Scientist (Chargé de recherche, CR) and associate	0
Other scientists (Chercheurs des EPIC et autres organismes, fondations ou entreprises privées)	0
Research supporting personnel (PAR)	0
Subtotal permanent personnel in active employment	0
Non-permanent teacher-researchers, researchers and associates	1
Non-permanent research supporting personnel (PAR)	1
Post-docs	0
PhD Students	5
Subtotal non-permanent personnel	7
Total	7

EVALUATION

Overall assessment of the team

The team has published several top papers in a highly competitive field of research. The publication chosen for emphasis in the evaluation documentation, i.e. from *Nature Catalysis* in 2019, is an outstanding piece of work, which is conceptually and practically innovative. The team has also initiated a process of valorisation of their works. It is very active in the training of young researchers (from MSc to postdoctoral fellows) and in the promotion of science among non-scientists directly and through social networks.

Strengths and possibilities linked to the context

Attractiveness

The team is scientifically very strong and offers good opportunities for growth. It investigates complex catalysis processes, where more than one catalytic cycle may be interlinked via a common species. While catalysis, in general, is a growing field, the coupling of multiple catalytic steps, as is done in nature, for example, by polyketide synthases, is a field just appearing on the horizon of organometallic chemistry. It promises to deliver yet greater selectivity and yet more efficient construction of complex molecules than had been previously imagined.

Production

The team is publishing high-quality papers in top-tier journals (*Science*, *Nature Catalysis*, *JACS*, etc.). The quantitative output is good for the small size of the group (18 papers in the period according to the Web of Science). Prof. Dydio has received several awards lately (Guy Ourrion Prize, Dream Chemistry, and Bürgenstock JSP fellow). The visibility of the team is good with about 20 invited conferences.

Inclusion in society

Catalysis provides a natural interface to industry. Prof. Dydio already has a productive collaboration on industrial catalysis, where his work makes a practical difference. Notably, patent application, collaborative agreement of a technology acceleration transfer company, and strong contacts with industrial companies (Solvay, Eastman) have been realized.

Weaknesses and risks linked to the context

Attractiveness

The field is highly competitive, and Prof. Dydio needs to expand his program to keep up with his competitors. Additional financial resources should be invested. Indeed, up to now the studies of the team are mostly financed by local grants through the future investment programs PIA (labex and idex), which is a weakness and a possible risk for the future.

Production

The field is highly competitive, with the primary production being peer-reviewed papers, and the secondary production being industrial collaborations. While Prof. Dydio has done well in both areas, his team needs to grow significantly in size and reach to maintain a leading position in the international context. Especially the industrial collaboration requires more depth of interaction with corporate partners, which means more resources, and more manpower.

Inclusion in society

It is very important that catalysis researchers have a view on what industry is doing. They should not duplicate industrial corporate research, and the only way to stay ahead is to stay engaged. Prof. Dydio should be encouraged to develop further contacts with industry so that he can maintain a realistic calibration of his research.

RECOMMENDATIONS TO THE TEAM

Considering what has been said above, the team is recommended to continue its successful path, which undoubtedly will lead to a higher international visibility and a further growth, both scientifically and with respect to financial resources.

Team 10: Laboratory of catalytic chemical synthesis

Name of the supervisor: Mr Amir Hoveyda

THEMES OF THE TEAM

The team is active in the field of organic synthesis, in particular homogeneous catalyst development based on the organometallic chemistry of inexpensive and abundant metals (molybdenum, copper and tungsten). It has developed some of the most frequently used catalysts for alkene metathesis and has discovered, among others, methods for the Z-selective metathesis, kinetic resolution, and stereoselective synthesis of trisubstituted alkenes and alkenyl halides. The team has also applied these methodological developments for the synthesis of complex natural products of biological relevance.

CONSIDERATION OF THE RECOMMENDATIONS OF THE PREVIOUS REPORT

Not applicable. The team leader joined ISIS only in 2019 and was not evaluated by the previous evaluation committee.

WORKFORCE OF THE TEAM

Permanent personnel in active employment	
Professors and associate professors	0
Lecturer and associate lecturer	0
Senior scientist (Directeur de recherche, DR) and associate	0
Scientist (Chargé de recherche, CR) and associate	0
Other scientists (Chercheurs des EPIC et autres organismes, fondations ou entreprises privées)	0
Research supporting personnel (PAR)	1
Subtotal permanent personnel in active employment	1
Non-permanent teacher-researchers, researchers and associates	2
Non-permanent research supporting personnel (PAR)	5
Post-docs	0
PhD Students	3
Subtotal non-permanent personnel	10
Total	11

EVALUATION

Overall assessment of the team

The research conducted by the team is at the forefront of organic synthesis in combination with organometallic chemistry and focuses on the use of earth abundant transition metals. The team leader is an outstanding scientist and one of the leaders in the alkene metathesis arena. His research team has developed some of the most-often used alkene metathesis catalysts that are useful for the construction of substituted alkenes. This work has made a great fundamental impact in the practice of organic synthesis, simplifying the access to complex molecular structures.

Strengths and possibilities linked to the context

Attractiveness

The team is very active in the combined fields of organic synthesis and catalysis, where it has made outstanding contributions. The team collaborates with other top scientists in this field, such as Profs. Richard Schrock and Ken Houk. In addition to his laboratories at ISIS, the team leader heads a research group at Boston College in the USA. In 2022 the team leader was awarded a prestigious ERC Advanced grant for the stereoselective synthesis of substituted alkenes by metathesis reactions.

Production

The team leader is a productive and highly cited researcher with a strong track record of impactful publications in top journals (mainly *Nature*, *Science*, *Nature Chemistry*, *J. Am. Chem. Soc.* and *Angew. Chem. Int. Ed.*). Some of the publications of his team are the result of collaborations with the above-mentioned top- scientists. The publication record in the period under assessment continued to be outstanding and there is no decline in activity.

Inclusion in society

The research conducted by the team in synthetic methodology and organometallic catalyst design has clear applications in the realm of medicinal chemistry, particularly in drug discovery. In addition, the chemistry developed by the team can be applied in materials research and fine chemicals synthesis. Several organometallic catalysts developed by the team are now commercially available and are widely used in research laboratories all over the world. The team leader is the co-founder of the XiMo company, now a subsidiary of the German company Verbio, which produces some of the metathesis catalysts developed by him at the ton-scale. The whole team is very active in bringing the results of his scientific studies to society in the form of lectures at international symposia. All these endeavours show that interactions of the team with industry and society are strong.

Weaknesses and risks linked to the context

Attractiveness

The team is at the forefront of chemical synthesis and the team leader has a high international visibility. The fact that the activities of the team leader are split between two laboratories in Boston and Strasbourg is more a strength than a weakness. The committee recommends him to continue his successful path.

Production

The publication record in the period under assessment is outstanding. There are no clear weaknesses or risks for the future.

Inclusion in society

The team is very active in bringing the results of his scientific outcomes to society and industry in the form of patents, spin-off companies, and lectures at international symposia. There are no weaknesses or risks for the future.

RECOMMENDATIONS TO THE TEAM

Prof. Hoveyda's research team is leading in catalyst design in the field of alkene metathesis. His research program is very creative, highly ambitious and certainly will continue to make a significant impact in the field of organic synthesis in the future. The committee recommends him to continue his successful path. Further support for his research program is highly recommended.

Team 11: Laboratory of exotic quantum matter
 Name of the supervisor: Ms Shannon Whitlock

THEMES OF THE TEAM

Prof. Whitlock is an experimental physicist who joined the University of Strasbourg in 2017 and ISIS in 2019. In a very short period, he has set up a group working on quantum optics and ultracold atoms, focusing on the control of quantum dynamics and on the emergence of complex structures. By now the team is among the leader on quantum simulations with cold Rydberg ensembles, as it is witnessed by a number of excellent research works. Furthermore, the group is a mainstay of the activities of Strasbourg related to the establishment of a center for quantum technologies. The group has strong links with leading scientists worldwide. At ISIS it has established a very productive collaboration with the group of Prof. Guido Pupillo.

CONSIDERATION OF THE RECOMMENDATIONS OF THE PREVIOUS REPORT

Not applicable. Prof. Whitlock joined ISIS after the publishing of the previous evaluation report.

WORKFORCE OF THE TEAM

Permanent personnel in active employment	
Professors and associate professors	1
Lecturer and associate lecturer	0
Senior scientist (Directeur de recherche, DR) and associate	0
Scientist (Chargé de recherche, CR) and associate	1
Other scientists (Chercheurs des EPIC et autres organismes, fondations ou entreprises privées)	0
Research supporting personnel (PAR)	0
Subtotal permanent personnel in active employment	2
Non-permanent teacher-researchers, researchers and associates	0
Non-permanent research supporting personnel (PAR)	0
Post-docs	1
PhD Students	3
Subtotal non-permanent personnel	4
Total	6

EVALUATION

Overall assessment of the team

The team has successfully established a prominent position in the experimental arena of quantum simulations. This was possible, among other things, because the team leader took an original research direction and implemented this experimentally remarkably well. To be particularly mentioned is the simulation of quantum cellular automata and the observation of the characteristic features of self-organized criticality using Rydberg atoms. These contributions are of outstanding quality and highly original. At the same time, the team leader is very much engaged in establishing a strong research infrastructure in the field in which he actively works. In this connection he closely collaborates with Prof. Guido Pupillo to make Strasbourg an emerging center of excellence for quantum technologies.

Strengths and possibilities linked to the context

Attractiveness

The field of research of the team completes and extends the research activities at ISIS. It matches the institute's objectives and has boosted its impact by providing visibility in the field of quantum optics, many-body physics, and quantum information communities. Within a short time, the team leader has managed to set up a research group that attracts talented graduate students and postdocs from France and all over the world. The acquired funding over the latest years is impressive. The research activities of the team have been disseminated through conferences and lectures by the team leader and by activities on social media. The attractiveness of the team is very high, especially considering that it is relatively young.

Production

In the last years the team has chosen a very original and impactful research focus and published a good number of high impact papers. The studies of the team are very solid, insightful, and original, and the journals in which the results are published are of high impact. The scientific production of the team is in line with its size. The committee values that the team prefers quality of publications over quantity.

Inclusion in society

The team is very active in the dissemination and transfer of knowledge outside of the academic environment. In addition to divulgation activities, the committee appreciates the projects of the group with industrial partners (BASF and IBM). These also include training networks (MOQS and QUSTEC), which programmatically involve internships of PhD students in industry and, vice versa, academic training of young researchers working in companies. It is to be noted that Prof. Whitlock coordinates the EFET training program, supported by the Quantum Flagship's Quantum Technology Education Coordination and Support Action. Special mention should be made of the activities of the Whitlock group for the project aQcess, which involves the establishment of a quantum computing platform in France. This is an extraordinary service to the scientific community and to society, which is highly appreciated by the committee.

Weaknesses and risks linked to the context

Attractiveness

The committee did not see any weaknesses or risks.

Production

The committee did not identify any weaknesses or risks.

Inclusion in society

The involvement of ISIS, and especially of this team and the team of Prof. Whitlock, in the long-term perspective of the aQcess project is not clear to the committee.

RECOMMENDATIONS TO THE TEAM

The research team is conducting excellent research in the field of experimental quantum physics and is successful in terms of scientific production, attractiveness, and funding. Moreover, the team is very active and successful in developing and establishing research and technological infrastructures. The committee especially values that the team managed in a short period of time to reach a leading position in the arena of experimental quantum simulations. The committee recommends the team to continue its successful path. In the coming years the team leader should receive all possible support for his program.

Team 12: Laboratory of molecular function and design
 Name of the supervisor: Mr Marco Cecchini

THEMES OF THE TEAM

This team is active at the interface of life sciences and materials science. By using state-of-art molecular simulations, it tries to provide a quantitative interpretation of fundamental phenomena at the molecular level, ranging from molecular recognition (molecular binding) processes and molecular self-assembly to the allosteric regulation of functional proteins.

CONSIDERATION OF THE RECOMMENDATIONS OF THE PREVIOUS REPORT

Not applicable. This research group was not evaluated in the previous assessment.

WORKFORCE OF THE TEAM

Permanent personnel in active employment	
Professors and associate professors	0
Lecturer and associate lecturer	0
Senior scientist (Directeur de recherche, DR) and associate	0
Scientist (Chargé de recherche, CR) and associate	0
Other scientists (Chercheurs des EPIC et autres organismes, fondations ou entreprises privées)	0
Research supporting personnel (PAR)	0
Subtotal permanent personnel in active employment	0
Non-permanent teacher-researchers, researchers and associates	0
Non-permanent research supporting personnel (PAR)	0
Post-docs	0
PhD Students	0
Subtotal non-permanent personnel	0
Total	0

EVALUATION

Overall assessment of the team

The prediction of molecular self-assembly by modelling and computer simulations is still an unsolved problem, particularly in the context of advanced materials design. To address this issue the team has established a theoretical framework to enable first-principle predictions of molecular self-assembly, which is nice. The scientific production of the team is proportionate to its research potential and the papers are of high quality, showing that the group values quality over quantity. The team leader has been able to acquire several national and international grants, especially European, which is laudable. Also, his top-level scientific collaborations with other groups deserve appreciation.

Strengths and possibilities linked to the context

Attractiveness

The team leader is a recognized expert in the development of adapted computational approaches, based on all-atom molecular dynamics, which provides a unique opportunity to monitor with atomic resolution the time evolution of the behavior of molecules. The statistical analysis of these single-molecule "experiments" eventually allows for a quantitative understanding of molecular function. The team explores and re-explores by theoretical and computational approaches the principles of chemical design, all the way from small organic compounds to complex nanomachines. Examples of the studies conducted by the team include the mechanism of operation and modulation of channel receptors, the functioning of biological motors and the calculation of the free enthalpy of binding of molecules and their self-assembly on surfaces.

Production

A very positive point is the collaboration of the team with partners of the highest international level, which are among the most influential players in the field of self-assembly at surfaces and interfaces. This leads to high quality papers in top journals. The production of the group is good and in line with the size of the group.

Inclusion in society

Compared to the previous evaluation period (< 2017), in which the team had no contacts with non-academic partners, they are now part of the ITI CSC Industrial Partners Program, and the skills of the team have been presented to BASF, SOLVAY, and GIVAUDAN at the first CSC partners meeting in July 2021. Furthermore, the team is developing products for the socio-economic world, as two former PhD students have recently been integrated in Pharma companies in France (Iktos & Bayer). Finally, it is worth mentioning that the team leader made a major contribution to the field of neuropharmacology by setting up the Glycine Receptor Allosteric Ligand Library (GRAL), which is the first database of allosteric modulators of a human synaptic receptor with a structural annotation based on their binding to the receptor site.

Weaknesses and risks linked to the context

Attractiveness

Dr. Marco Cecchini joined ISIS in 2010 and left this institute in 2017. His research group was relatively small compared to other groups at ISIS. Nevertheless, he has made major contributions to the research activities of ISIS. The committee does not see real weaknesses or risks.

Production

After Dr. Cecchini made his most important achievement in 2016, i.e. the formulation of a general theoretical framework for a first-principle interpretation of molecular self-assembly at surfaces and at the liquid-graphite interfaces (*PCCP* 2016, 18, 31480, *ChemPhysChem* 2016), a decrease of peer-reviewed articles has been visible, but these articles are still published in top-tier journals. The team leader should keep an eye on his production levels in the future.

Inclusion in society

Even though the research activities of the team are exploratory and fundamental in nature, the group has made substantial efforts to interact with the socio-economic world. Nevertheless, these activities could be further improved, as noticed by the team leader himself.

RECOMMENDATIONS TO THE TEAM

The committee regrets that Dr. Cecchini left ISIS in 2017. The institute may consider hiring a person with a similar profile as Dr. Cecchini in the future.

CONDUCT OF THE INTERVIEWS

Dates

Start: October 5, 2022 at 8.30

End: October 6, 2022 at 17.00

Interview conducted on-site and online

INTERVIEW SCHEDULE

October 5th

08 :30	08 :50	Welcome of the committee
08 :50	09 :00	Presentation of the committee
09 :00	09 :30	Presentation by the Director (assessment and trajectory)
09 :30	10 :00	Discussion
10 :00	10 :10	Debriefing
10 :10	10 :15	Coffee break
10 :15	10 :30	Presentation by Paolo Samorì (assessment)
10 :30	10 :45	Discussion
10 :45	11 :00	Presentation by Thomas Ebbesen (assessment)
11 :00	11 :15	Discussion
11 :15	11 :30	Presentation by Jean-Marie Lehn (assessment)
11 :30	11 :45	Discussion
11 :45	11 :55	Presentation by Thomas Hermans (assessment)
11 :55	12 :05	Discussion
12 :05	12 :15	Presentation by Vladimir Torbeev (assessment)
12 :15	12 :25	Discussion
12 :25	12 :50	Debriefing
12 :50	14 :00	Lunch break (meal tray)
14 :00	14 :15	Presentation by Joseph Moran (assessment)
14 :15	14 :30	Discussion
14 :30	14 :45	Presentation by Amir Hoveyda (assessment)
14 :45	15 :00	Discussion
15 :00	15 :10	Presentation by Pawel Dydio (assessment)
15 :10	15 :20	Discussion
15 :20	15 :35	Presentation by Guido Pupillo (assessment)
15 :35	15 :50	Discussion
15 :50	16 :05	Presentation by Shannon Whitlock (assessment)
16 :05	16 :20	Discussion
16 :20	16 :40	Debriefing
16 :40	16 :50	Coffee break
16 :50	17 :10	Discussion with Team leaders (without management team)
17 :10	18 :40	Debriefing

October 6th

08 :45	09 :00	Welcome of the committee
09 :00	09 :30	Interview with engineers and technicians (ITA, Biatss)
09 :30	10 :00	Interview with doctorates and post-doctorates
10 :00	10 :30	Interview with researcher and teaching staffs (without management team)
10 :30	10 :45	Debriefing
10 :45	11 :00	Coffee break
11 :00	11 :45	Interview with supervisory institutions (CNRS and Unistra)
11 :45	12 :00	Debriefing
12 :00	13 :30	Lunch break (meal tray)
13 :30	14 :00	Interview with the management team
14 :00	17 :00	Final debriefing of the committee

PARTICULAR POINT TO BE MENTIONNED

Because of Covid 19, two committee members, Ms Chantal Andraud and Ms Giovanna Morigi participated by video. The second day (October 6th), Ms Giovanna Morigi did not participate.

GENERAL OBSERVATIONS OF THE SUPERVISORS

Monsieur Éric Saint-Aman
Directeur du Département d'évaluation de la recherche
HCERES - Haut conseil de l'évaluation de la recherche et
de l'enseignement supérieur
2 rue Albert Einstein
75013 PARIS

Strasbourg, le 14 décembre 2022

Objet : Rapport d'évaluation DER-PUR230023195 - ISIS - Institut de science et d'ingénierie supramoléculaires.

Réf. : RB/FF/N° 2022-309

Rémi Barillon

Vice-Président Recherche,
formation doctorale et science
ouverte

Cher Collègue,

Affaire suivie par :

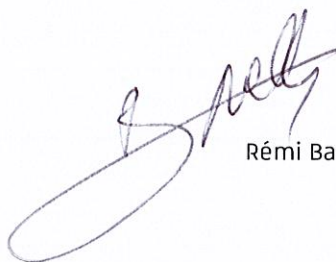
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L'université de Strasbourg vous remercie ainsi que tous les membres du comité HCERES pour le travail d'expertise réalisé sur l'unité de recherche « Institut de science et d'ingénierie supramoléculaires » (ISIS – UMR 7006)

Nous n'avons aucune observation de portée générale à formuler sur le rapport d'évaluation transmis.

Je vous prie d'agréer, Cher Collègue, l'expression de mes cordiales salutations.



Rémi Barillon

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