Industry interactions of the electronic structure research community in Europe

A survey carried out on behalf of the Psi-k network and the CECAM-UK-JCMaxwell Node

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Executive Summary

Psi-k [http://www.psi-k.org/] is a network of the European *ab initio* research community. This report explores the interactions of the academic Psi-k community with industry. The evidence presented is mainly based on a semi-quantitative survey and interviews of network members, and the analysis stands in the context of a prior report on the economic impact of molecular modelling [1] as well as of a recent study into Science-to-Business (S-2-B) collaborations [2] in general.

Pertinent findings of the economic impact report were that the dominant electronic structure method, Density Functional Theory (DFT), is the most widely accepted 'molecular modelling' method and that it has become established in the electronics industry. Also of significance are the more than average growth in the number of patents which include DFT, and the growing interest in the potential of modelling in a wider circle of researchers in industry.

The S-2-B study [2] emphasized the key role of the Principal Investigator (PI) in establishing and maintaining a satisfactory relationship, and the importance to industry of 'soft' objectives relative to outcomes with hard metrics.

All Psi-k board, working group and advisory group members, a total of about 120 people were invited to take part in the study, and 40 people responded, representing more than 400 scientists from 33 different institutions in 12 European countries. While it is acknowledged that this group will to some extent pre-select those with industry collaborations, the result that 90% of respondents work with industry is still significant. Main industry sectors of the collaborators are materials, electronics, automotive and aerospace and software. Density functional theory is almost always used in industry collaborations but classical and higher level theory also feature strongly.

It was noted that the Psi-k network represents some of the most widely used electronic structure codes in the world. In fact, all electronic structure codes available in the leading commercial packages (see Table 2) originate from Europe and are used at a few hundred industrial sites worldwide.

Psi-k groups that work with industry collaborate on average with 2-3 companies, typically on a long term basis. It is interesting that small groups are just as likely to collaborate with industry as larger ones, and also with roughly the same number of companies. There is however a correlation between the number of collaborating companies and the number of alumni in industry positions, which is consistent with the observation of the S-2-B study that the role of the PI and the depth of the relationship are the dominant factors.

Considering the different forms of interactions, informal interactions dominated, followed by collaborative projects, consultancies and training. Collaborative projects were reported by 75% of respondents with on average one such project per team per year. Nearly 60% of respondents had consultancy and contract research projects, with an average of one such engagement per research team every 1-2 years. Training was least frequent but still more than 40% of respondents had training interactions in the last three years.

The main drivers for industry to collaborate are seen to be the expertise of the PI and access to new ideas and insights. As measures of success, new insights dominate followed by achieving breakthroughs in R&D. On the other hand, despite a clear ROI, cost saving is not generally the driver for collaborations. Impact was often achieved by unveiling mechanisms that could explain observations on a fundamental level and that had previously not been known or properly understood. The new insights thereby helped to overcome long standing misconceptions, leading to a completely new way of thinking and research direction. Similarly, electronic structure calculations helped to scrutinize certain concepts or aspects of engineering models. Less frequently so far seems to be the determination of input parameters for these models. However, the ability of simulations to screen a large number of systems, which would be prohibitively expensive if done experimentally, also plays an important role.

The above evidence and mechanisms of success indicate that the Psi-k network is largely in line with S-2-B collaborations in general [2], for example in terms of the relationships, importance of PI and the typical 'soft' measures of success.

On the other hand we can also see significant opportunities for further improvement. There is sincere interest as well as unmet need in industry. On the one hand, the gap between industry requirements and what can be delivered by today's theories and simulations is widely acknowledged. On the other hand, there is plenty of evidence that important and impactful topics can be addressed with current methods. However it takes a lot of time, effort and translation skills to identify and act upon these. Despite some activities by the network to further the exchange with industrial research, there is still too little common ground in terms of interactions, interests and language to develop the personal relationships that were found to be crucial for engagements between academics and industry.

However, we see evidence of successful mechanisms that can be built upon. These include utilising multiscale modelling approaches as not only a scientific endeavour but also as an opportunity to build a bridge in terms of communication and relationships. Also, relationships with industry at the level of Ph.D. training seems to be an effective mechanisms not only to train scientists with the relevant skills and understanding but also to build long term relationships between the academic centres and industry. Similarly, centres of excellence that are by their nature set up with industry involvement provide visibility and help to build relationships, although with the proviso [2] that the single investigator can be the critical determinant.

Introduction

There has been very significant growth in the field of electronic structure and molecular modelling in the last 30 years, and its impact in general terms can be traced from the code authors through to a range of beneficiaries in industry and society [1]. In particular, the size of the *ab initio* research community has recently been estimated [3] based on the number of distinct authors of *ab initio* papers as at least 22,000 worldwide, of which half are based in Europe!

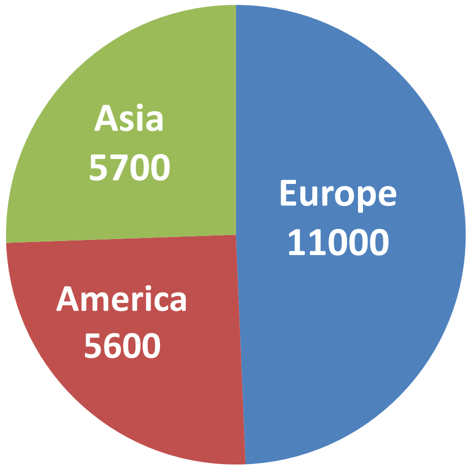


Figure 1: Estimate of the number of scientists active in the electronic structure field. The number for Asia is an underestimate in that it only includes China, Japan, Korea, Taiwan and Singapore. From Ref [3].

The general impact of the efforts of this community as well as of molecular modelling researchers has been discussed in an earlier study [1]. Pertinent points which underline the industrial impact of electronic structure research include:

- Density Functional Theory (DFT) is the most widely accepted amongst the quantum, atomistic and molecular modelling methods.
- In the electronics industry electronic structure experts have become part of “the team”.
- The software industry has emerged from a ‘hype cycle’ into a phase of sustained growth.
- There has been a significant rise in the number of patents which include DFT, also as a proportion of the number of patents within the respective fields.
- Electronic structure calculations may form a small but significant part of engineering workflows that have been shown to yield substantial returns on investment.

However, it was also pointed out that significant gaps and barriers remain, in particular

- Many phenomena of industrial interest remain very hard to capture well at least in standard electronic structure calculations.
- There is a need for more people with a skill for translating between industrial problems and what can be done with atomistic simulation technology, supported by technology managers with the knowledge, perception and position to commit resources to simulation which are at least comparable to experimentation.

Psi-k network

In this report we look at the industry collaborations of people in the Psi-k network of the European *ab initio* research community which includes more than 2000 scientists.

Its objectives and activities as described on the network website include the following:

- Psi-k supports European research and researchers in *ab initio* computational modelling of materials and aims to further Europe's leading role in the application of computational modelling from first principles to materials science.
- "Psi-k research" covers structures, properties and processes in all types of materials at the atomic level and in nanometre-scale structures, studied by *ab initio* quantum mechanical computer simulation.
- Psi-k activities include the continuous development of computational methodology at all levels, from e.g. more efficient codes to the inclusion of many body theories, all based on *ab initio* methods.

The scope and size of activities of the European electronic structure community is remarkable. Psi-k activities are represented by 17 working groups and subgroups ranging from correlated systems, magnetism and multiscale methods to real material properties, nanoscience, surface science, catalysis, corrosion and biological systems. Psi-K organises a number of events and symposia including a large conference with global reach every five years. The last such event in 2010 was attended by more than 1000 scientists [4], with the previous one in 2005 attended by 560 scientists [5]. Also, Psi-k members and codes play a crucial role in the European Theoretical Spectroscopy Facility, which offers significant opportunities for industrial collaboration.

Science-to-Business collaborations

A recent publication [2] provides some useful general background to so-called Science-to-Business (S-2-B) collaborations including a short review of literature on industry-university interactions. Points of interest from prior studies include:

- Industrial R&D managers attach very little importance to measurable performance-metrics, such as licensing and patents [6].
- "Economically important 'outputs' of university research" [6] are described as soft outputs, such as:
    - scientific and technological information that improves industry R&D efficiency;
    - the use of equipment and instruments by industry;
    - skills or human capital of students and researchers;
    - collaborations of scientific and technological competences for the diffusion of new knowledge.

Types of knowledge exchange can be classified according to their level of intensity [7]:

- Transmission: I have sent my research results to private firms, government agencies and other users outside the academic milieu;
- Presentation: I have been invited to present my research results to groups and organisations who could make direct use of them;

- Effort: I have been asked to sit in on working groups that were involved in direct efforts to apply new knowledge including my own research;
- Consultation: I have provided consulting services to private firms, government agencies or organizations associated with my research field;
- Use: The use of my research results has contributed to the development of new or improved goods or services;
- Business activities: I am involved in business activities outside laboratories that are related to my research activities;
- Commercialisation: Others have attempted to commercialise the results of my research.

D'Este and Patel [8] proposed the following grouping of interaction types into five categories

- Meetings and conferences, e.g. attendance at industry sponsored meetings.
- Consultancy work and contract research commissioned by industry, typically not involving original research.
- Creation of physical facilities with industry funding, e.g. campus laboratories, incubators and cooperative research centres, and setting up spin-off companies.
- Training company employees and postgraduate training in company, e.g. joint supervision of PhDs.
- Joint Research agreements involving research undertaken by both parties.

Their data on industry collaborations supported the above grouping as the activities were found to be largely non-overlapping, i.e. conceptually these five categories represent distinct forms of interaction.

Boehm et al [2] investigate the "process of establishing scientific–knowledge–commercialization collaborations" in further detail, in particular how and by whom such S-2-B collaborations are established and maintained. While previous work considered the motives to partner with universities from an industry perspective, Boehm at al looks at these issues from the perspective of all collaborating partners on a project.

For the initiation of S-2-B relationships, it is found that "both industry and university partners initiate collaborations". The PIs play a crucial role in the initiation of these relationships, while Technology Transfer Organisations (TTOs) "are hardly ever seen as the initiator or the point of contact for industry partners."

According to Boehm et al, the two main reasons for industry to initiate collaboration are: (a) a special interest in a research area or topic to solve a problem; and (b) the reputation of the PI. Furthermore the study points out the importance of personal relationships: "Industry partners and academics alike outline that knowing people beforehand through personal relationships, having worked with them before or where industry partners are alumni of a university contributes to the initiation of collaborative projects."

Successful S-2-B collaborations with repeated projects establish a long term relationship between the partners which are characterized by a clear understanding of each other's roles and mutual satisfaction. The latter is related to the expectations of the collaboration which are evaluated in terms of the quality of the interaction with the other parties as well as deliverables and service.

Expectation management and taking the requirement of both sides into consideration is key to success: "poorly considered or imbalanced objectives are likely to result in a negative affective condition even in a situation where the project objectives are met."

Regarding the reasons and expectation for a collaboration on the industry side, nearly 70% of industrial partners "explained that being part of collaborations is important not only for access to knowledge but also for generating and evaluating better ideas. On the other hand, academics also acknowledge the value of access to 'knowledge of real needs'."

In conclusion the study highlights the importance of long-standing engagements with companies. Infrastructures and programmes that support and promote building these relationships play an important role. Examples according to Boehm et al [2] and references therein include industry Ph.D. programs and Centres of excellence due to the concentration of a number of PIs in one location. However, building partnerships at the PI level remains the "critical determinant" [2].

Survey of the Psi-K network

In the following we present results of a survey of the European Psi-k research community concerning interactions with industry. Over a period of three months, 122 members of the Psi-k network across Europe were contacted and 40 people from 33 different institutions in 12 countries provided input. 33 of those provided answers to the survey: see Appendix A for the questions and Appendix B for an overview of answers. Also, 16 people provided input in phone interviews, which will be discussed in the section on ***Evidence and analysis from phone interviews*** below.

The survey was completed by 33 people from 28 distinct organisations in the following countries: Austria (2), Belgium (3), Finland (2), France (2), Germany (6), Ireland (1), Italy (1), Portugal (1), Spain (1), Sweden (3), The Netherlands (1), and United Kingdom (10). They represented 86 senior staff, 123 post-docs and 190 PhD students, i.e. a total of about 400 scientists.

85% of respondents were Professors, and 15% Group Leader. They provided answers for their groups. Most groups consist of two senior and post-doctoral staff and four students, with the largest groups having up to ten senior staff, and 10-20 post-docs as well as 10-20 PhD students.

Regarding collaborations with industry, we note that response to the survey will to some extent pre-select those in the network that actually have industry collaborations. In fact, the interviews with some of the board members indicated that many groups, including a number of very large groups have no industry collaboration at all. On the other hand, this is to be expected in a field which includes fundamental theory and method development which will only become of relevance to industry over a 10-20 year time frame, but is very important in order to address the gaps and shortcomings of the models.

With that proviso, we find that 90% of respondents collaborated with industry in some form in the last three years. 70% had interactions in government funded projects and two thirds worked with companies outside of government projects. On average respondents collaborate with two companies and a maximum of five.

Overwhelmingly the collaborations are with European companies. Only 5 respondents had any collaborations outside of Europe, and only 2 had the majority outside of Europe. In other words, in 80% of cases all collaborating companies were in Europe, and in the remaining 20% there was still a majority of collaborations with European companies. Before we discuss further details about the types of interaction with industry, the following section provides an overview of the research topics and industry application areas of the respondents.

90% of respondents collaborate with industry.

Research applications and industry sectors of collaborations

Research application areas of the respondents reflect the more materials property oriented working groups as would be expected from a group which is largely involved in industrial collaborations.

Most frequently mentioned application areas include:

- Semiconductors and microelectronics applications.
- Energy materials (incl photovoltaics and thermo-electrics).
- Oxides, metals, alloys and their chemo-mechanical behaviour.
- Graphene, carbon nanotubes and other low dimensional materials.

This was followed by:

- Catalysts.
- Coatings and surface properties.
- Ceramic compounds.
- Biomaterials.
- Functional Materials.
- Polymer and elastomer materials.

In individual cases the following were mentioned: quantum dots, transition metals, aqueous solutions, high pressure applications, supramolecular self-assembly, magnetic materials, nuclear materials, nanoparticles, organic and biological materials and systems.

Researchers study the above fields by determining properties at the electronic structure level, in particular (in order of frequency with which they were mentioned):

- Structural parameters.
- Density of states, band structure/gap.
- Total energy and formation enthalpy.
- Optical and dielectric properties.
- Charge correlation and transfer, conductivity.

Also mentioned were spectroscopy, defects, excited states and excitation energies, elastic properties, reactions, transition states, magnetic properties, spin density and correlation, phonon spectra, hyperfine fields, electric field gradients, work functions and diffusion constants.

Collaborations take place with a wide range of industries, with the majority in materials, electronics, automotive and aerospace, rather than chemicals and pharmceuticals, as would be expected from a physics and materials based network (see Figure 2).

Main industry sectors of collaborations are materials, electronics, automotive and aerospace and software.

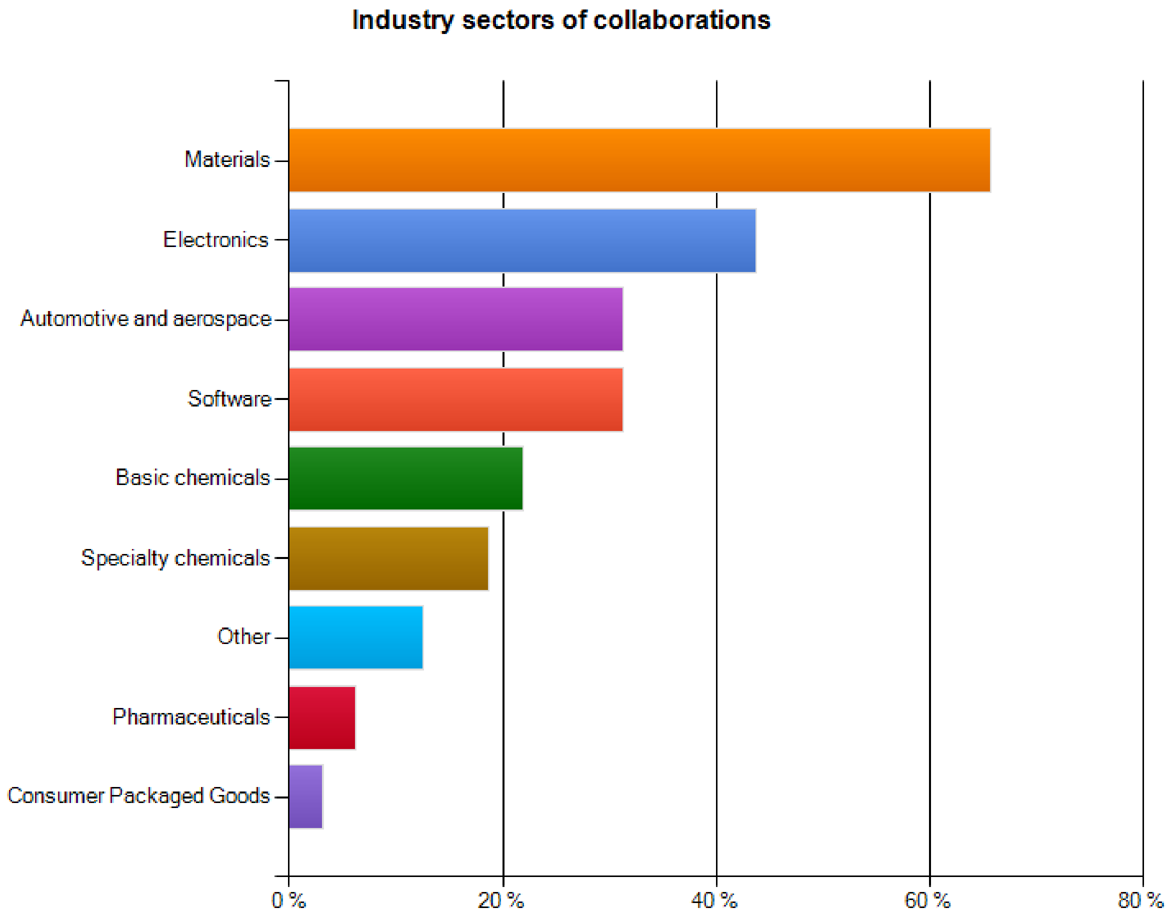


Figure 2: Industry sectors of the collaborating companies. "Other" industry sectors include: Extraction of oil, gas, minerals and ores, photovoltaics and nuclear power.

The dominant application topics of industry collaborations reflect the main industry sectors shown in Figure 2. The list of topics shown in Table 1 is topped by semiconductors and micro-electronics applications as well as devices, followed by energy materials research and the behaviour of metals and alloys. It was mentioned quite frequently that these collaborations are aimed at searching for new materials and properties using a kind of knowledge based design approach. Not surprisingly, some relatively new areas such as low dimensional materials which feature quite high on the research list are lower down the list of industrial research topics. Biomedical and drug design were mentioned as occasional applications as well as general consulting.

Incidentally these topics are consistent with the patenting activity involving widely used electronic structure calculations with codes such as ABINIT, CASTEP, GPAW, Quantum ESPRESSO, VASP and Wien2K. A patent search using Patentscope (http://patentscope.wipo.int/) shows 63 international (Patent Cooperation Treaty) patent applications since 2005 which are overwhelmingly in category H01L (Semiconductor Devices; Electric Solid State Devices), followed by C01B (Non-Metallic Elements; Compounds thereof) and H01M (Processes or Means (e.g. Batteries) for the Direct Conversion of Chemical Energy into Electrical Energy).

Table 1: Application topics of industry collaborations

Topic	Mentions
Semiconductors, microelectronics applications, devices, sensors etc	9
Energy materials (incl photovoltaics and thermo-electrics)	7
Metals and alloys, grain boundaries, chemomechanical behaviour (incl fracture)	7
New materials search/screen, knowledge based design, new materials properties, structure-property insights	6
Catalysts	3
Software development	3
Impurities and defects	2
Coatings and surface properties, corrosion	2
Fuels and lubricants	2
Graphene and CNT and other low dimensional materials	1
Functional Materials	1
Polymer and elastomer materials incl membranes and seals	1
Mineral extraction	1

Software development and application in industry

As expected from members of the Psi-k network all respondents and their groups were found to be modelling users. Most respondents (85%) are also active as authors, typically involved in the development of density functional methods (see Figure 3). However, there is also significant activity across a wide range of methods from classical to higher level theory, as well as hybrid QM/MM and other multiscale methods, visualization and analysis tools, and dislocation dynamics.

The methods that respondents use in industry collaborations largely reflect those also used in original research, except for a more dominant use of density functional methods (see Figure 3). Nevertheless about one third of respondents use either higher level or classical methods occasionally in industry projects.

Density functional theory is almost always used in industry collaborations but classical and higher level theory also feature strongly.

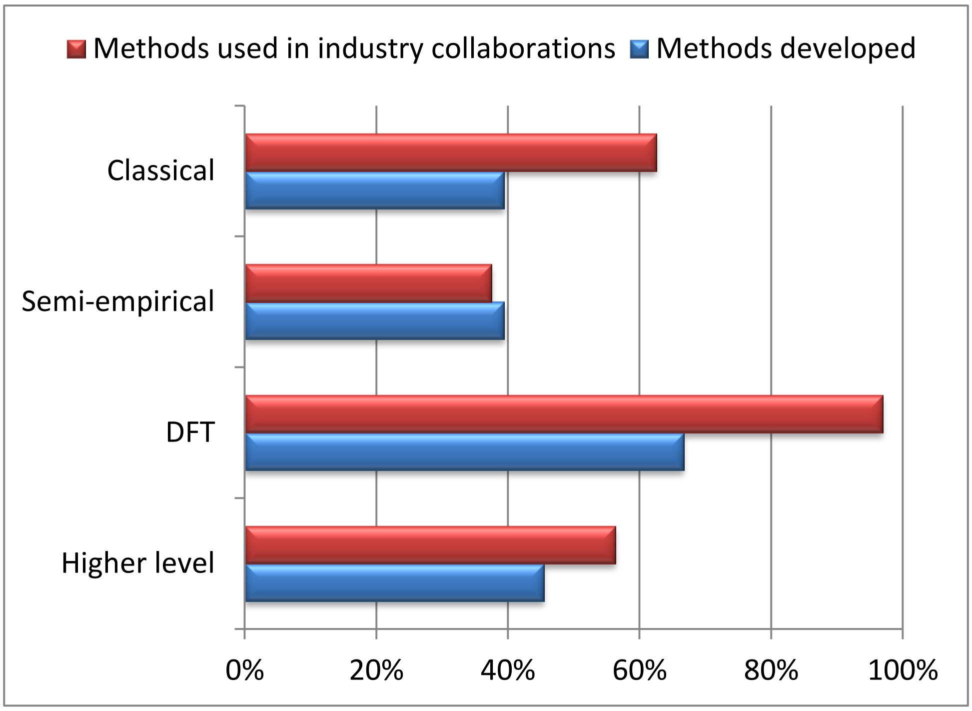


Figure 3: Percentage of respondents that developed a range of different methods shown in blue, and used different methods frequently or occasionally in industry collaborations, shown in red.

In this context, we also note that the Psi-k network represents some of the most widely used electronic structure codes in the world (see a non-comprehensive list in Table 2), including the two commercially most significant codes, CASTEP and VASP.

Table 2: Electronic structure codes developed by researchers in Europe linked to the Psi-k network. A number of codes are integrated into the open source Atomic Simulation Environment (ASE) as well as into commercial software packages as shown in the second column.

Code name	**Software/Integration**
ABINIT	Scienomics MAPS , QuantumWise ATK and ASE
ADF/BAND	SCM BAND
BigDFT	
CASTEP	Accelrys Materials Studio and ASE
CP2K	
CPMD	
DACAPO	ASE
DFTB and DFTB+	Accelrys Materials Studio, ASE and SCM
Exciting, Elk	ASE
FHI-Aims	ASE
Fleur	ASE
GPAW	ASE and QuantumWise ATK
Hb Hotbit	ASE
Octopus	Nanohub
ONETEP	Accelrys Materials Studio and ASE
Quantum ESPRESSO	PWgui and ASE
SIESTA	ASE
VASP	Materials Design Medea and ASE
Wien2K	

The related collaboration of Psi-K academics with software companies was reflected in the replies from 3 out of the 33 respondents, who reported 'software development' as one of the activities of the collaboration and in some cases significant royalties as a benefit. Also, a few companies were set up by members of Psi-k for doing code development as well as for industry [9].

Dissemination and use of these packages in industry is difficult to quantify, the two main reasons being that codes are either proprietary (e.g. BAND, CASTEP, VASP) and hence the figures about distribution are confidential, or codes are open source (e.g. ABINIT), which by its nature means that there is no register of licences.

Nevertheless it has been possible to obtain recent figures for some of the commercial codes, which show some growth relative to previously reported figures [9] which indicated that VASP is licensed to about 75 companies and the FLAPW code Wien 2k is licensed to about 50 groups in industry. In total, the picture remains that worldwide there are a few hundred industrial sites that access one of the electronic structure codes from the Psi-k network. Industrial application is by far the largest in the Far East, in particular Japan, with about 1/5th of all industry users in Europe.

Psi-k network represents some of the most widely used electronic structure codes in the world. Electronic structure codes integrated in the leading commercial packages originate from Europe and are used at more than 200 industrial sites worldwide.

Collaborations with Industry

The survey asked a number of questions about the quantity and quality of collaborations with industry, see questions 11-20 in ***Appendix A***: The Survey and corresponding answers in ***Appendix B***: Summary of survey responses. On average, respondents and their groups collaborate with two companies in government projects and with 1.4 directly. Considering just the respondents that have collaborations, the averages are 2.9 and 2, respectively. The maximum number is eight for government projects (probably due to EU collaborations) and six outside of government projects.

There are many long standing collaborations ranging from four months to more than twenty years, with an average of 6 years and a median of four years. The number of project renewals was on average three, ranging up to ten.

Project durations tend to be longer than one year, in line with academic research cycles (e.g. post-doc positions and research objectives). More than 85% of respondents were involved in industry collaborations that had an element of government funding, typically one or two over a three year period, with about 10% of respondents having a total of six!

In purely industry funded projects there are occasional shorter ones: about 20% of respondents had projects of less than a year in that timeframe. About 75% of respondents had industry funded projects without government funding in the last three years. Most had one or two, but 15% of respondents had four or more projects.

Academic groups that work with industry collaborate with 2-3 companies on average. Many collaborations are long term.

The survey does not show a correlation between the group size and the number of companies the group collaborates with as Figure 4 shows. There are significant fluctuations and differences between the groups, and while some large groups have more collaborations, there is no general trend.

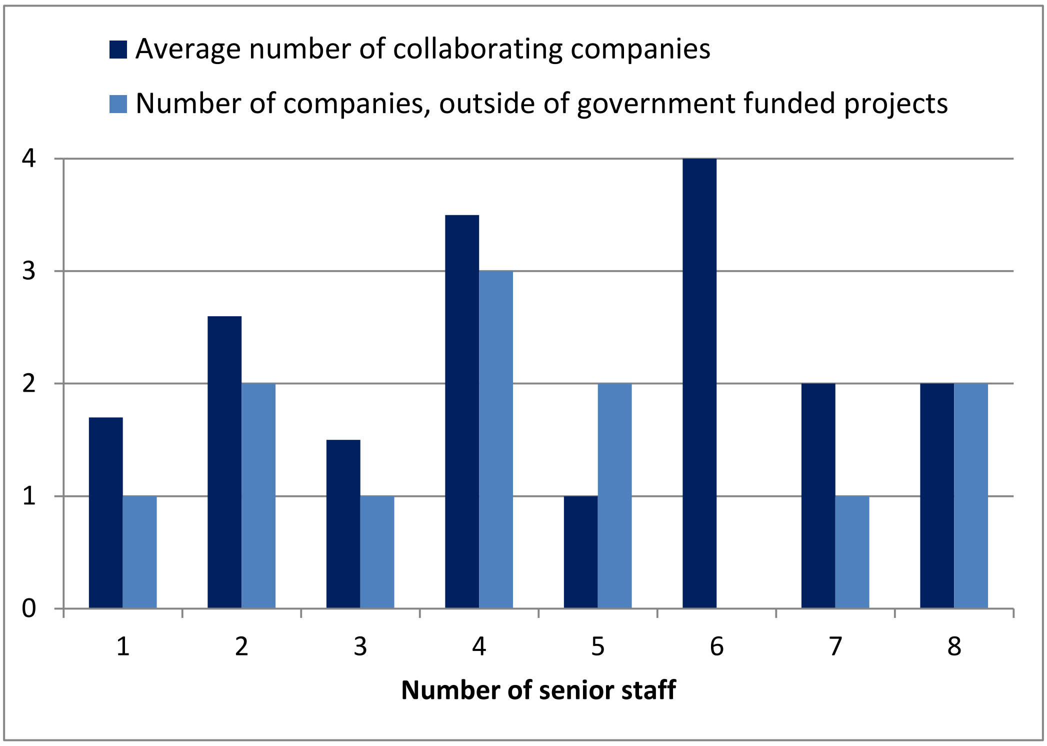


Figure 4: Industry collaborations for academic groups of different number of senior staff. Shown are the average number collaborating companies (Question 17 in Appendix A) and the collaborations in projects without government funding (Question 12).

Small groups are just as likely to collaborate with industry as larger ones, and also with roughly the same number of companies.

On the other hand, one can tentatively say that there is some correlation between the number of group alumni in industry and the number of companies that a group collaborates with, as shown in Figure 5. Of 23 respondents to the question, 17 had alumni in industry, with 44 of the 65 ex-students having taken up computational roles.

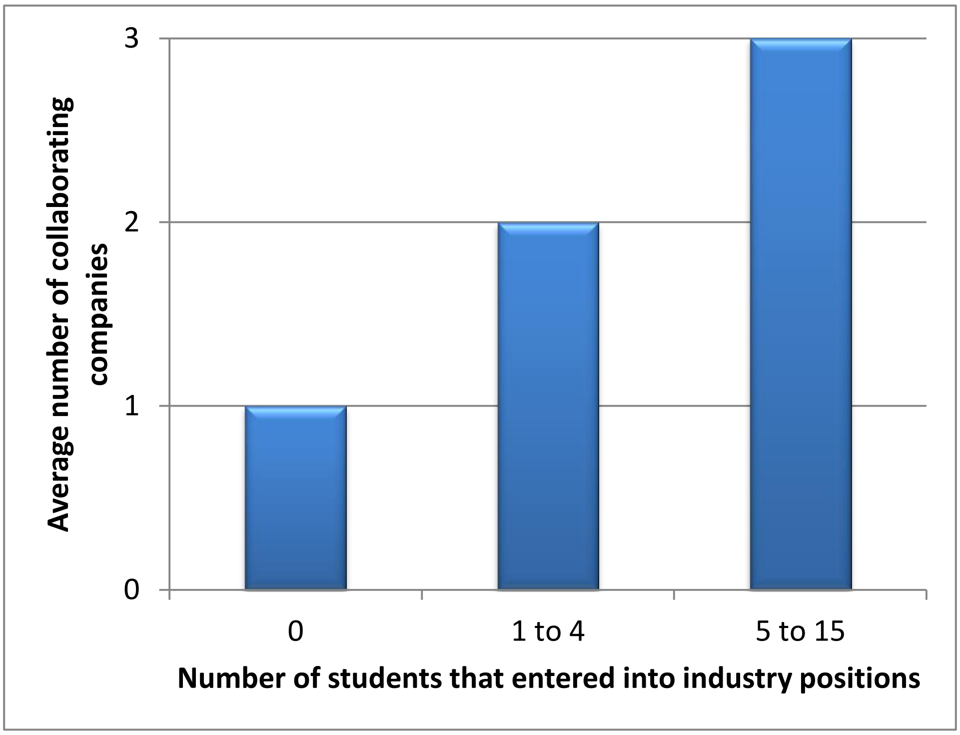


Figure 5: The average number of collaborating companies plotted against the number of students from a group that have taken jobs in industry.

These above findings are consistent with the findings of S-2-B collaborations in general in that the depths of the relationship plays a strong role, as indicated by long standing collaborations and alumni relationships more than by the size of the research group.

There is a correlation between the number of collaborating companies and the number of alumni in industry positions.

In order to elucidate the aspects of the relationships in further detail, survey participants were asked to consider their industry interactions along five categories largely based on those put forward by D'Este and Patel:

- Informal personal interactions
- Formal consultancy and contract research
- Collaborative research projects
- Training
- Setting up physical facility or spin-off company

The frequency of these types of interaction was measured, ranging from zero to on average more than four times a year (more than 12 times in three years). The matrix of responses (Table 3) and the chart in Figure 6 show that, not surprisingly, informal interactions dominate, with more than 40% of respondents having on average more than four such interactions per year. Across all respondents there are on average two informal interactions per Psi-k research team per year.

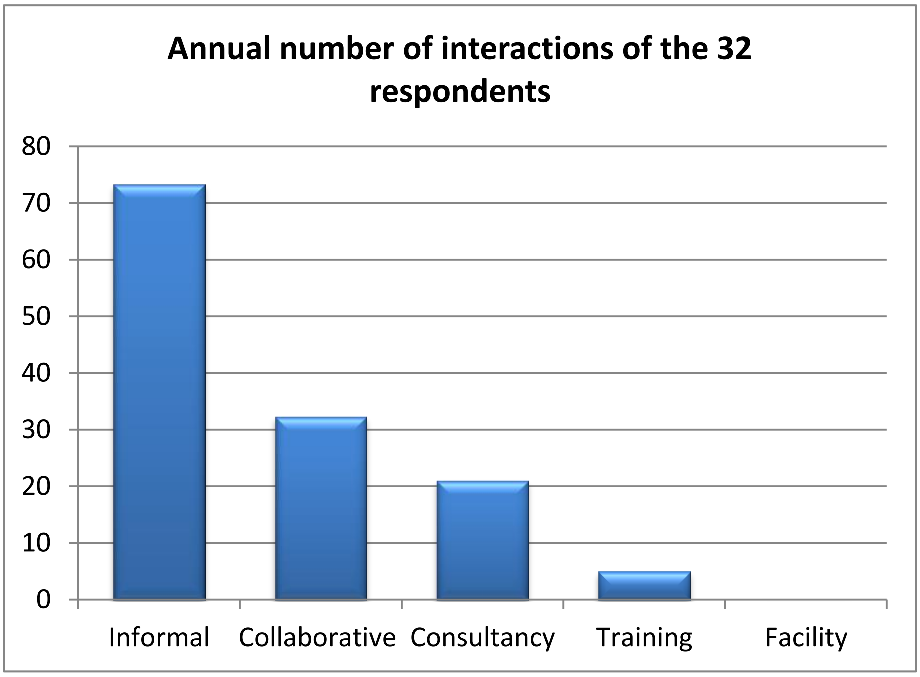


Figure 6: Annual number of interactions of the respondents in different categories

Collaborative projects were reported by 75% of respondents with on average one such project per team per year and more than twelve collaborative projects over a three year period in some groups.

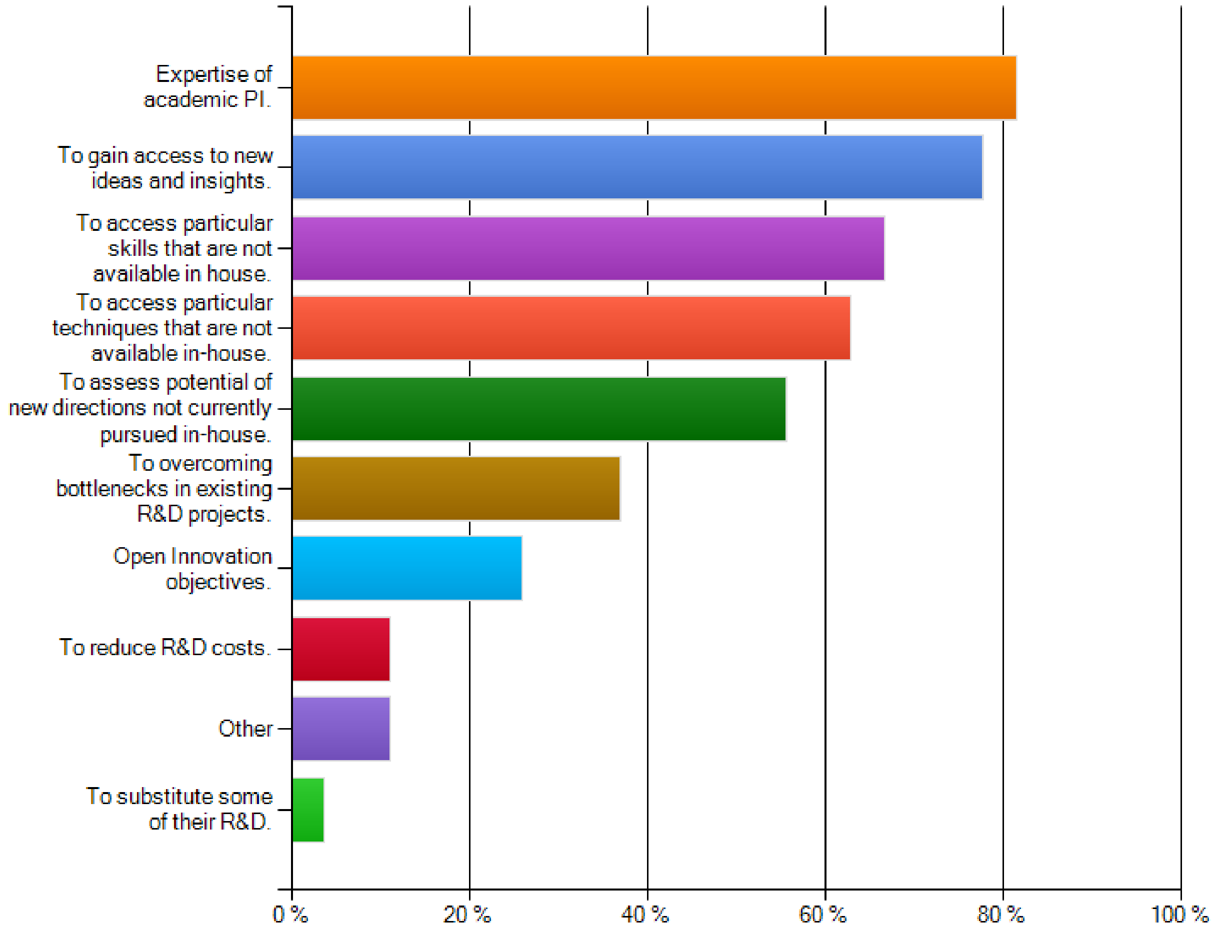
Nearly 60% engaged in formal consultancy and contract research, although the latter tend to be relatively infrequent. On average there is one such consultancy engagement per research team every 1-2 years. Training was least frequent but still more than 40% of respondents had training interactions in the last three years. On the other hand, none was involved in setting up facilities or spin-out companies.

Table 3: Frequency of interactions in different categories over a three year timeframe. The ranges with most respondents are shown in dark orange and the second most in light orange.

Category of interaction	0	1-2	3-6	7-11	>= 12
Informal personal interactions	10%	13.3%	16.7%	16.7%	43.3%
Formal consultancy and contract research	41.9%	35.5%	16.1%	3.2%	3.2%
Collaborative research projects	25%	40.6%	21.9%	3.1%	9.4%
Training company employees	58.6%	37.9%	3.5%	0%	0%
Setting up a a spin-off company etc	100%	0%	0%	0%	0%

Industry motivation and success criteria

The survey aimed to probe the reasons why industry enters and remains in collaborations with academics in the network. As shown in Figure 7 expertise of the PI and access to new ideas are regarded as the major factors for industry to enter into collaborations, followed by skills and techniques and the possibility to assess new directions. While also of some importance, overcoming bottlenecks and open innovation objectives play somewhat less of a role. Specific Return-on-investment (ROI) metrics such as cost reduction and substituting R&D are least important. Training of people and external funding were also mentioned as a reason to enter into collaborations.



Expertise of the PI and access to new ideas and insights are seen as the main drivers for industry to collaborate with academics in the Psi-k network. Hard ROI metrics are least important.

As measures of success (Figure 8), new insights dominate, followed by achieving breakthroughs in R&D. As will be discussed in more detail below, the interviews reflected this picture. For example it was remarked that overcoming bottlenecks of a strategic, long-term nature is an important driver for collaboration. There are cases where the company has kept on running into the same problem, and aims to address the issue at a fundamental level using modelling. The time scale of providing a solution is often less critical. Also, it was remarked that insights from theory and modelling have been successful in helping to steer experimentation and avoid dead ends. While there is a clear ROI in that, cost saving is not generally the driver for collaborations, at least not in the short term. Broadly these findings agree with the general picture from the Boehm S-2-B study [2] that in many ways the 'soft' outputs play a bigger role than measurable performance-metrics.

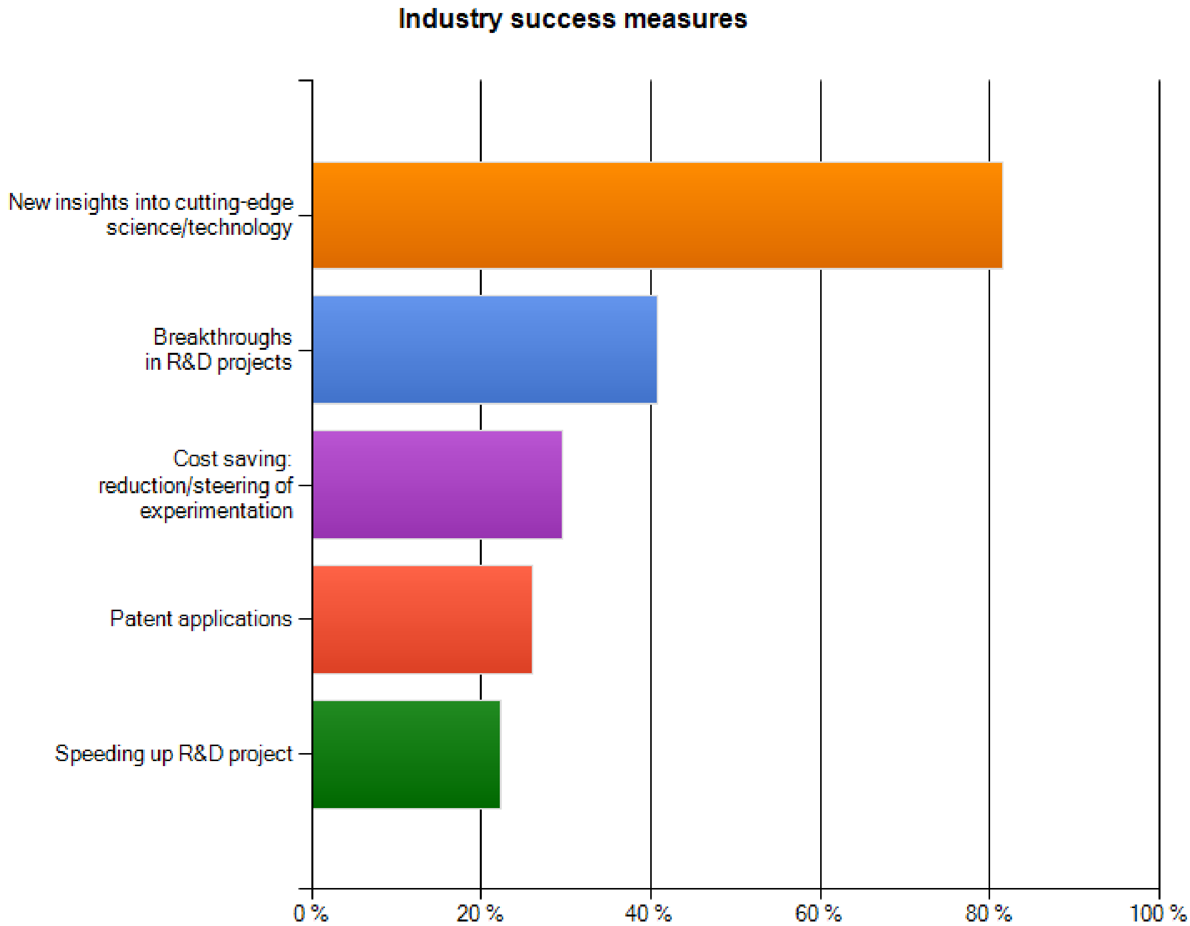


Figure 8: Percentage of respondents that selected different measures of success applied by industry to the collaboration.

Impact on industry R&D

Respondents described a number of success stories from which we can identify characteristics that are very much in line with the dominant measures of success shown in Figure 8. In many cases the success was about unveiling mechanisms that could explain observations on a fundamental level and that had previously not been known or properly understood. The new insights thereby helped to overcome often long standing misconceptions, leading to a completely new way of thinking and research direction. Similarly, electronic structure calculations helped to scrutinize certain concepts or aspects of engineering models. Less frequently so far seems to be the determination of input parameters for these models. In several cases the impact was achieved due to the ability of simulations to screen a large number of systems, which would be prohibitively expensive if done experimentally.

Typical application areas included failure mechanisms and coming up with directions for improvement, elucidation of conduction mechanisms, catalytic pathways, and tuning of optical and electronic properties. A number of ‘stories’ of impactful applications of *ab initio* methods are due to be published in a forthcoming Psi-k newsletter. Topics include

- *Ab initio* thermodynamics and statistical mechanics enabling the understanding of crystal growth and exploration of heterogeneous catalysis.
- Biochemistry applications such as the action of anti-cancer drugs.
- Crystal structure prediction supporting computational materials discovery.
- Computational mineral physics as a tool to understand planetary interiors.
- Device performance and functionality by studying transport on the nanoscale, half-metallic compounds (a new class of ferromagnets) and tunnelling magneto resistance.
- Energy applications such as photovoltaics.
- Theoretical spectroscopy, highly complementary to the respective experimental techniques for the study of matter and development of new materials.

Benefits for academia

Respondents overwhelmingly agreed that industry collaborations are beneficial to the academic process in that complex industrial problems often bring up requirements, trigger new method developments and provide ideas and focus on areas that require general advancement. However, the secrecy on the industry side is regarded sometimes to be a hindrance to making the most out of these opportunities.

The main points in response to Question 21 (see ***Appendix A***: The Survey) were:

- Publications: Since most of the industry interactions are research collaborations, publications are a key outcome, and most respondents noted several or many publications, including “high-impact publication with technological relevance”.
- Patents: while patenting activity was not regarded as a major driver, a quarter of respondents nevertheless reported patenting activity resulting from industry collaborations. This includes patent claims that do not explicitly mention that the research involved electronic structure modelling.

- New methods: about half of the respondents noted that new methods were developed as a result of the collaborations. In fact some of the responses noted that "new problem sets and driving capability is one of the main incentives", that these collaborations bring up questions that would not otherwise come up and that "one of these methods has attracted more than 100 citations".
- Students: It was noted that collaboration with industry not only helped with funding for studentships but has been important for providing relationships and much better insights for students.
- Income: About 10% of respondents reported in some cases substantial royalty income from software development and a similar number also substantial income from direct industry collaborations. In other cases collaborations with industry are simply regarded as part of a package that helps to secure government funding.

Evidence and analysis from phone interviews

In addition to the survey, phone interviews were conducted with sixteen academics from the Psi-k network, all professors and research group leaders, representing 12 organisations in five countries (Germany, UK, Finland, France and Switzerland).

A number of topics emerged from these interviews which highlight key aspects of Psi-k industry interactions:

- **Industry expectations and requirements**: there is sincere interest and need but in many cases a gap remains between requirements and what can be delivered.
- **Suitable topics, methods time scales**: while many important problems cannot be solved on time scales that are compatible with industrial research, there are plenty of topics which can be addressed with current methods. However it takes a lot of time and effort to identify these.
- **Developing successful relationships** with industry requires sustained effort and expectation management by the Principal Investigator (PI) but support structures also play a role.
- **Overcoming barriers**: there are significant gaps between the Psi-k community and industrial research, requiring translation mechanisms and efforts to facilitate collaboration.

Industry expectations and requirements

As was reported previously [1] there has been a significant growth in the number of so-called 'consumers of modelling', i.e. researchers that see a potential benefit of modelling even if they are not modelling users themselves. Consistent with the above picture are the following remarks by one of the board members of Psi-K: "Interest from industry in *ab initio* modelling has clearly grown over the past 10-15 years. Fifteen years ago, suggestions in that direction were met with a polite smile. Nowadays, there is sincere interest."

However, the question is how well the community can meet industry's needs and requirements. It was noted that widely publicized success stories from the field could give the impression that *ab initio* modelling can provide industry with their desired new material in a few years, leading to expectations that could often not be met. While quantitative answers are not always required, the predictive power of the method is still very important. Industry is after fundamental insights but also material parameters that are otherwise hard to get and even semi-quantitative data are valuable. Partly this requirement stems from the increased level of sophistication and detail of engineering models which require better insights and more parameters.

However, currently electronic structure methods are not generally robust enough to be integrated into engineering workflows by default. In fact, engineers were rarely mentioned as contact persons in industry collaborations. It was noted that in most cases just applying the simulation is not sufficient: a lot of understanding of the topic and the method as well as related interpretation of results is required. In general technology terms, one could say that electronic structure calculations are still not a 'stackable'technology, i.e. cannot yet perform the role of a component in a technology stack. One interviewee commented that in fact there is a crisis in the field because of this lack of accuracy.

As a result some companies withdraw from the technology while others retain a kind of observational involvement. There is general interest in industry to keep up to date with computational tools that could be of interest in the long term and there remains an expectation of long-term R&D cost savings resulting from the increased use of simulation in contrast to the ever more costly experiments and materials tests. Some companies invest in research collaborations with a view to increased output in the public domain (e.g. publications). The aim is to build research communities and help to attract public funding to help bridge the gap to higher levels of technological readiness.

Suitable topics, methods and time scales

In the meantime, not only expectation management is key but also matching methods and topics. As was expressed by one interviewee: "The bottleneck for new collaborations, as I experienced several times, is to define research questions that are simultaneously doable (for the computational scientists) and useful (from the industry point of view). Although there are for sure many such topics, it takes a real effort and many deep discussions to identify them."

Some respondents however also mentioned that the timescale for setting up and running meaningful simulations for complex systems was not compatible with the timescale of industry projects. Also, it was remarked that tackling these problems often required additional functionality in codes. While it might be possible to develop these, the time scale generally does not meet industry expectations: "Many problems in industrial materials development are too complex for today's electronic/atomistic structure simulation capability and capacity. Also, the time scales of electronic structure calculations and industry R&D are usually not compatible. That's not just the physical problem timescale but the time it takes to come up with meaningful results is too long (usually at least 6 months to 1 year)."

On the other hand, if an important, long-standing bottleneck has been identified, time to solve it becomes less of an issue. Two of the interviewees remarked that there are cases where the company has kept on running into the same problem again and again and is ready to take the time it take to address that at a fundamental level.

Developing relationships

Developing and sustaining relationships is a key factor in S-2-B collaborations in general [2], and there is plenty of evidence to support that from the interviews. Respondents commented that developing collaborations requires personal and colleague networks as well as substantial and sustained effort on behalf of the PI. One PI spent more than a week talking to R&D staff at an industry R&D site. While this amount of time and effort may be prohibitive for many academics, the interviews suggest that the more fruitful and longer term projects often involved a long lead time of building trust and relationships.

On the other hand, many academics in the Psi-k network don't collaborate with industry other than being in government funded projects more or less alongside each other. In fact there are some very large research groups in the network without any industry collaboration.

As was found by Boehme et al, the personal chemistry between the investigators often lies behind success or failure. However, this is also a limiting factor in a situation where industrial R&D often lacks people that have been trained in electronic structure methods as also shown by the survey finding that only in a quarter of cases the main contact in industry was a computational scientist.

Overcoming barriers

Successful collaborations and impact on industrial problems have been achieved where effort has gone into building relationships as well as identifying suitable topics. However, we have seen that there are very significant barriers in the way.

In industry, there is a lack of critical understanding of the first principles modelling methodology, of its present-day capabilities and challenges. Most companies do not have computational scientists at the atomic scale, and hence often lack the expertise to translate their needs into what can be done by modelling at the electronic structure level. Also, the experience is that senior management lacks relevant understanding of the issues and opportunities of applying first principles modelling. In other words there is too little in-house competence to help define what could and should be done both strategically and tactically.

That means there is a community building issue with unexploited possibilities. Some industry R&D groups might have a need but don't know that there is a possible solution. Publications don't help since most companies lack the expertise and bandwidth for understanding relevant academic research results in relevant modelling and simulation. Hence there is a big need for "translation".

At the same time, established quantum chemistry groups in industry tend not to interact with materials science and engineering. Electronic structure calculations as represented by Psi-k (can) provide an important role in filling that gap. Examples include: heterogeneous catalysis (in contrast to homogeneous (quantum chemistry) [10,11]; and high performance ceramic coatings (in contrast to additive molecules).

Involvement in multiscale modelling activities helps in overcoming these barriers. Experience of interviewees has been that it first of all helps to build the relationship to different communities and overcome language barriers. Also, the readiness to apply whatever modelling technique may be suitable is clearly important, rather than just sticking to electronic structure calculations. However, people found that it in most cases their actual project contributions ended up purely at the electronic structure level anyway. The multiscale picture just served to make the link. One of the reasons is that industry already has groups working at the coarse grained level, which means that the multiscale picture provides a point of contact. Also, they require improved insights and ideally input data (even if only semi-quantitative) from the fundamental level.

However, the current setup of the electronic structure community is not generally conducive to building these bridges. For example, it was remarked that the community of PIs tends to meet in conferences and symposia with little industrial participation. As conferences and meetings attended by industrial R&D and by Psi-k academics don't overlap very much the opportunity for personal contact is relatively weak. Also other mechanisms to initiate collaborations are not well established. Wherever such initiatives or mechanisms exist, more and stronger collaborations are formed. Examples include: Fraunhofer Society initiated collaborations in Germany, institutes such as the Max-Planck-Institut für Eisenforschung (MPIE) which have been set up with strong industry involvement, and Doctoral Training Centres in the United Kingdom that include industry participation as an essential element.

Conclusions and Outlook

There is plenty of evidence of strong interactions of significant parts of the Psi-k community with industry. In line with Science-to-Business collaborations more widely, building collaborations requires focussing on the relationships first, providing expertise and if appropriate the translation to electronic structure calculations. Since not all problems lend themselves directly to electronic structure calculations, a flexible approach based on fundamental understanding, and appropriate levels of modelling has been shown to lead to success. This however can only be delivered by people and organisations with a broader perspective.

There is hence a need for 'translators' both on a personal and organisational level. More effort is needed to train industrial R&D scientists and educate their managers in *ab initio* materials modelling. On an organisational level, the Fraunhofer Institutes as well as specific MPIs in Germany fulfil that role. In the UK there is some indication that Doctoral Training Centres which require strong involvement from industry help to bridge the gap. On the other hand it is interesting that EU collaborative projects were not generally seen as a conduit for building stronger industry-academia collaboration. Likewise, schemes that just provide electronic structure codes and hardware for use by industry are not sufficient since with a few exceptions industry is not in a position to benefit from that. A promising scheme on the other hand is that provided by the European Theoretical Spectroscopy Facility, which offers significant opportunities for industrial collaboration.

Networks such as Psi-k clearly have a strong role to play here as well. Today, Psi-k performs mostly an internal network function: connecting people, job announcements, conferences. While this is an important function for the field which Psi-k has clearly performed with great success, structures and organisations that take on more of an external, ambassadorial and "translation" role are also required. In the United States for example the Materials Genome Initiative and the Materials Project have led to a much wider appreciation of the capabilities and potential for impact [12].

Finally, further attention is needed to move the field up the scale of Technology Readiness Levels. This cannot be achieved without the different actors (i.e. the research community as represented by Psi-K, industry as well as government agencies such as the Technology Strategy Board in the UK and similar agencies in Europe) working together to support the Principal Investigators that are "the critical determinant" [2] for success.

Appendix A: The Survey

Over a period of 3 months (mid July to mid October 2013) an online survey was conducted using SurveyMonkey. 122 people in the network were contacted (mostly board members and working group members as well as members of the Scientific Advisory Committee), of which 34 took the survey and phone interviews were conducted with 15 people.

Survey Questions:

About you and your group

1. Please provide your name and institution.

Name

Institution

Country

2. What is your role?

- Professor
- Group leader
- Post-doc
- Other

Other (please specify)

3. How many members does your group have currently?

Senior Staff

Postdocs

Graduate Students

4. Considering the involvement with theory and modeling, how many people in your group fall into the respective categories? For people involved in more than one activity, just count them into each relevant category.

Code authors

Modeling users

Consumers of model results

Methods and applications

5. What types of modeling method do you and your group develop?

- [ ] Higher level theory
- [ ] Density functional theory
- [ ] Semi-empirical methods including DFTB
- [ ] Classical simulation
- [ ] Other

Please specify Other

6. What types of 'observables' and properties do you determine? Observables and properties refer to the quantities that are calculated directly from the simulation.

Frequently

Occasionally

Rarely

7. What fields of application does your group work on in general? These include types of materials and target applications of materials, e.g. alloy, semiconductors, displays etc.

Frequently

Occasionally

Rarely

Industry Collaborations

8. What modeling methods do you and your group use in industry collaborations?

	Frequently	Occasionally	Never
Higher level theory	◯	◯	◯
Density functional theory	◯	◯	◯
Semi-empirical methods including DFTB	◯	◯	◯
Classical simulation	◯	◯	◯
Other	◯	◯	◯

Please specify Other

9. Considering industry collaborations, what types of applications is your group involved in?

Freqently

Occasionally

Rarely

10. What industry sectors do the companies you work with represent?

- ☐ Basic chemicals
- ☐ Specialty chemicals
- ☐ Materials
- ☐ Electronics
- ☐ Automotive and aerospace
- ☐ Pharmaceuticals
- ☐ Consumer Packaged Goods
- ☐ Software
- ☐ Other

Please specify Other

11. How frequently have you been engaged in the following industry interactions in the last 3 years?

	0 times	1-2 times	3-6 times	7-11 times	>= 12 times
Informal personal interactions (i.e. not involving a signed agreement)	◯	◯	◯	◯	◯
Consultancy and contract research (formal, with specific objectives)	◯	◯	◯	◯	◯
Research funded by industry (typically collaborative research projects)	◯	◯	◯	◯	◯
Training company employees	◯	◯	◯	◯	◯
Setting up a physical facility for industry or a spin-off company	◯	◯	◯	◯	◯
Other	◯	◯	◯	◯	◯

Please specify Other

12. In the last 3 years, how many different companies have you and your team worked with (i.e. had some sort of funding from)?

In government funded projects

Without government funding

13. In the last 3 years, how many different industry funded projects of what different duration has your team been involved with? (Count different projects with the same company separately).

	With government funding	Without government funding
up to 3 weeks long		
3 weeks to 3 months long		
3 months to 1 year long		
Longer than 1 year		

14. What is the job function of your main contact in these industry projects?

	In most cases	Sometimes	Rarely	Never
R&D manager	◯	◯	◯	◯
Lab scientist (e.g. characterization)	◯	◯	◯	◯
Computational scientist	◯	◯	◯	◯
Engineer (chemical/material/electronics)	◯	◯	◯	◯
Other	◯	◯	◯	◯

Please specify Other:

Measures of success

15. What is your longest standing industry collaboration?

Duration in months:

Comment:

16. How many renewals/projects have you had with the same company?

Number of projects:

17. How many companies do you collaborate with on average at a given time?

18. What percentage of these companies are in Europe?

19. What are the main reasons for your industry collaborators to enter into projects?

- ☐ Expertise of academic PI.
- ☐ To gain access to new ideas and insights.
- ☐ To access particular skills that are not available in house.
- ☐ To access particular techniques that are not available in-house.
- ☐ To overcoming bottlenecks in existing R&D projects.
- ☐ To assess potential of new directions not currently pursued in-house.
- ☐ To substitute some of their R&D.
- ☐ To reduce R&D costs.
- ☐ Open Innovation objectives.
- ☐ Other

Please specify Other expectations

20. What measures of success are applied by companies?

- ☐ Patent applications
- ☐ New insights into cutting-edge science/technology
- ☐ Breakthroughs in R&D projects
- ☐ Speeding up R&D project
- ☐ Cost saving: reduction/steering of experimentation
- ☐ Other ROI measures (please specify)

Please specify Other Return on Investment (ROI) measure

21. What have been the key success outcomes from your perspective? Please comment and provide numbers where relevant.

Publications	
Patent applications	
Royalties	
New methods developed	
Students trained	
Funding for research	
Effect on research assessments	
Other (please comment)	

22. How many students have been trained in your group in the last 5 years that then went on to work in industrial R&D?

Entered into computational roles	
Other roles in industrial R&D	

23. Please provide examples and success stories.

Many thanks for taking part in this survey!

Appendix B: Summary of survey responses

About you and your group

Question 1: Please provide your name and institution.

The survey was completed by 33 people from 28 distinct organisations in the following countries: Austria (2), Belgium (3), Finland (2), France (2), Germany (6), Ireland (1), Italy (1), Portugal (1), Spain (1), Sweden (3), The Netherlands (1), United Kingdom (10)

Question 2: What is your role?

85 % of respondents were Professors, and 15% Group Leader.

Question 3: How many members does your group have currently?

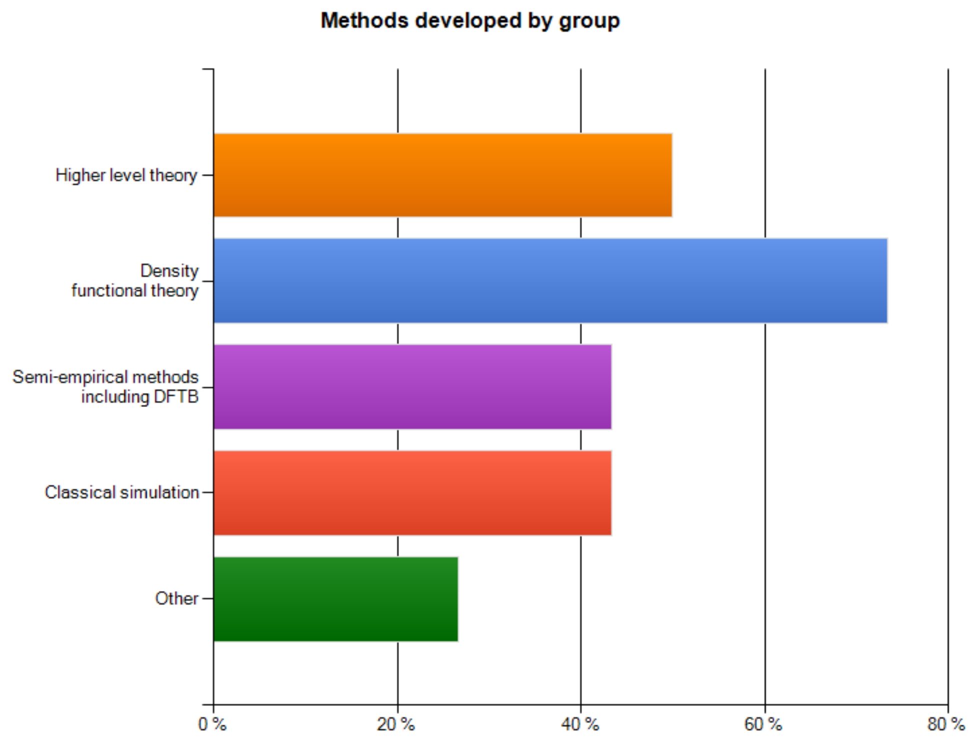
Most groups have 2 senior and post-doctoral staff and 4 students, with the largest groups having up to 10 senior staff, and between 10-20 post-docs as well as 10-20 PhD students.

Question 4: Considering the involvement with theory and modeling, how many people in your group fall into the respective categories?

All group members are modelling users, and 85% are also active as authors.

Methods and applications

Question 5: What types of modelling method do you and your group develop?



"Other" includes: hybrid QM/MM and other multiscale methods, visualization and analysis tools, as well as dislocation dynamics.

Question 6 : What types of 'observables' and properties do you determine?

Frequent

Observable	mentions
structural parameters	14
density of states, band structure/gap	9
total energy and formation enthalpy	9
optical and dielectric properties	7
charge correlation and transfer, conductivity	7
spectroscopy	4
defects	4
excited states, excitation energies	4
elastic properties	3
reactions, transition states	3
magnetic properties	3
spin density and correlation	2
phonon spectra	1
hyperfine fields	1
electric field gradients	1
work functions	1
diffusion constants	1

Question 7 : What fields of application does your group work on in general?

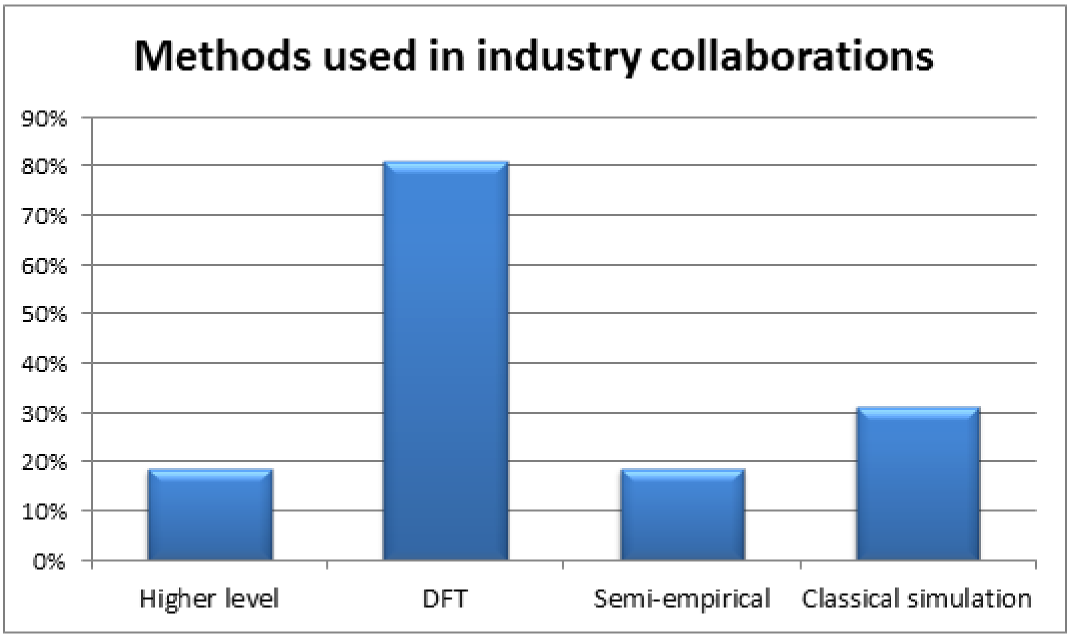
Frequent

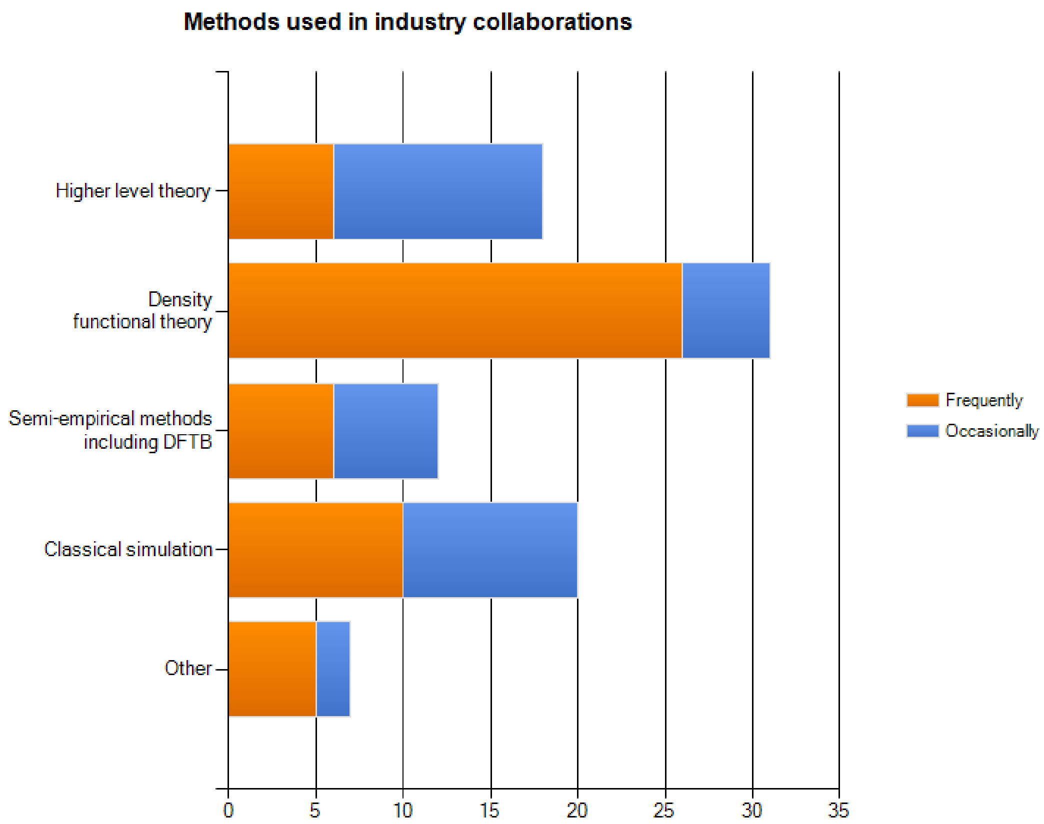
Application	Mentions
Semiconductors and microelectronics applications	11
Energy materials (incl photovoltaics and thermo-electrics)	11
Oxides	10
Metals and alloys and their chemomechanical behaviour	8
Graphene and CNT and other low dimensional materials	7
Catalysts	4
Impurities and defects	3
Coatings and surface properties	3
Ceramic compounds	3
Biomaterials	3
Functional Materials	2
Polymer and elastomer materials	2
Quantum dots	1
Transition metals	1
Aqueous solutions	1
High pressure applications	1
Supramolecular self assembly	1
Magnetic materials	1
Nuclear materials	1
Nanoparticles	1

Occasional and rarer applications were largely similar, except for a number of groups mentioning occasional and rare applications in organic and biological materials and systems.

Industry collaborations

Question 8 : What modeling methods do you and your group use in industry collaborations?

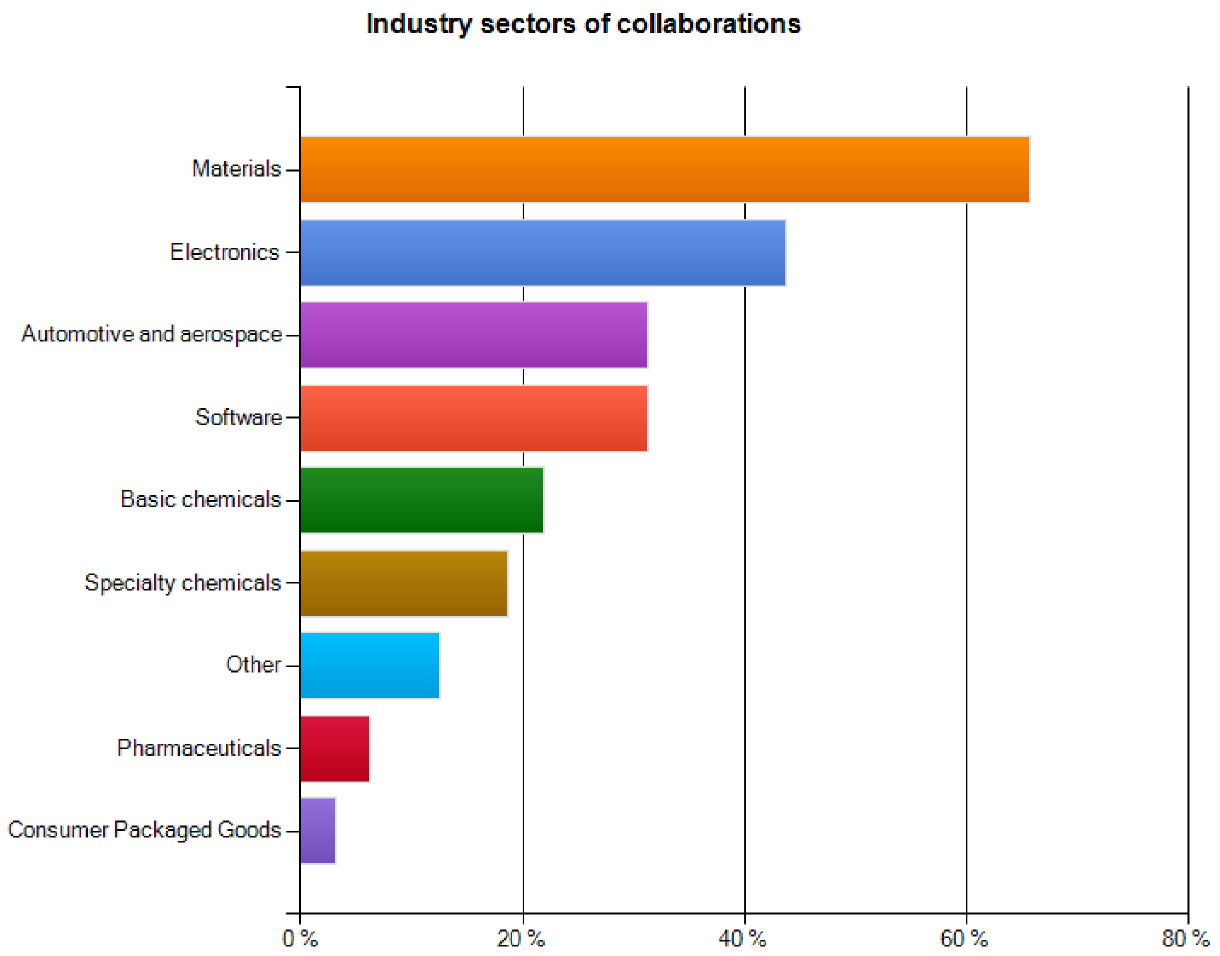




Question 9: Considering industry collaborations, what types of applications is your group involved in?

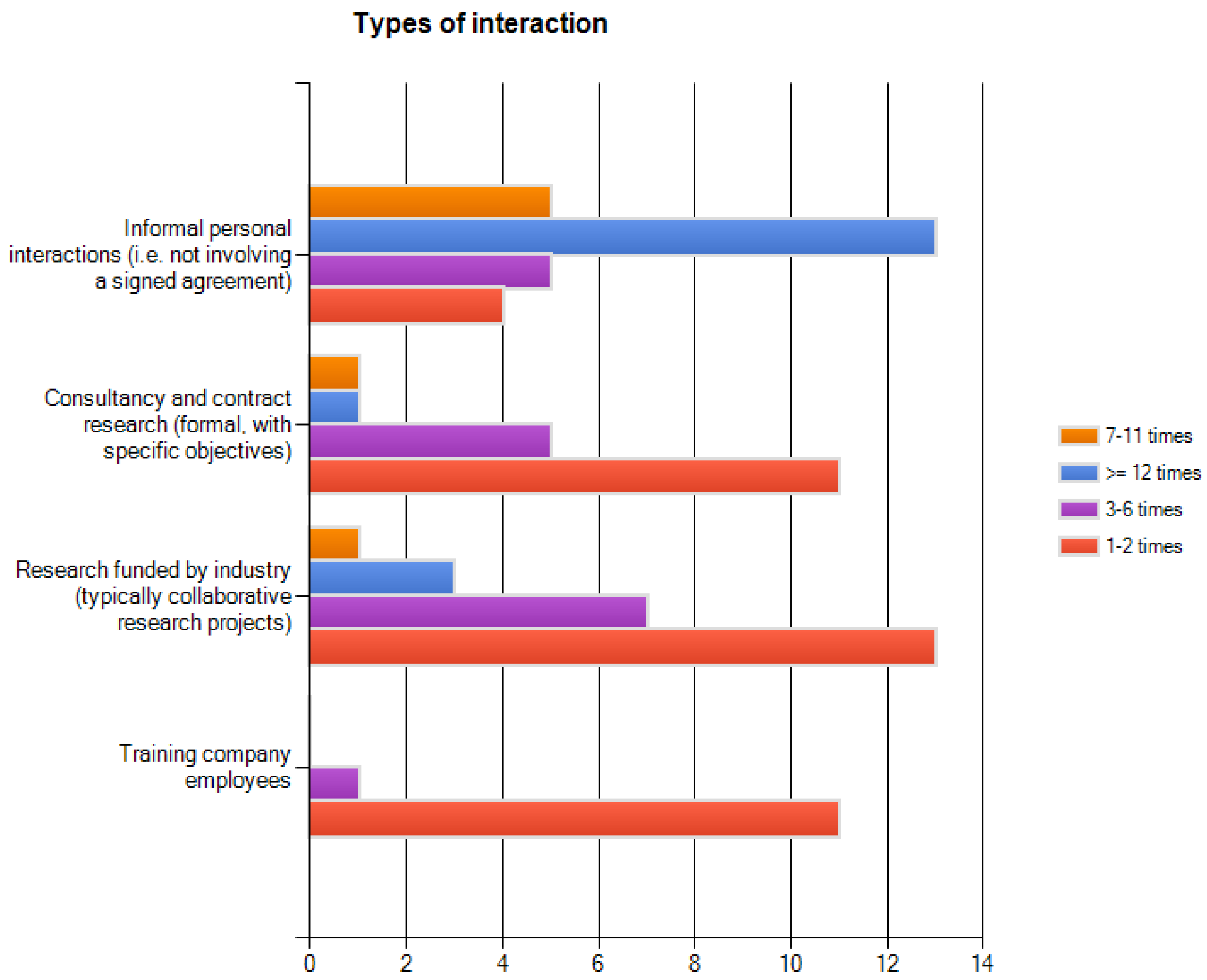
Topic	Mentions
Semiconductors, microelectronics applications, devices, sensors etc	9
Energy materials (incl photovoltaics and thermo-electrics)	7
Metals and alloys, grain boundaries, chemomechanical behaviour (incl fracture)	7
New materials search/screen, knowledge based design, new materials properties, structure-property insights	6
Catalysts	3
Software development	3
Impurities and defects	2
Coatings and surface properties, corrosion	2
Fuels and lubricants	2
Graphene and CNT and other low dimensional materials	1
Functional Materials	1
Polymer and elastomer materials incl membranes and seals	1
Mineral extraction	1

Question 10: What industry sectors do the companies you work with represent?



Question 11: How frequently have you been engaged in the following industry interactions in the last 3 years?

	0	1-2	3-6	7-11	>= 12	Total
Informal personal interactions	10% 3	13.3% 4	16.7% 5	16.7% 5	43.3% 13	30
Formal consultancy and contract research	41.9% 13	35.5% 11	16.1% 5	3.2% 1	3.2% 1	31
Research funded by industry, collaborative research projects	25% 8	40.6% 13	21.9% 7	3.1% 1	9.4% 3	32
Training company employees	58.6% 17	37.9% 11	3.5% 1	0% 0	0% 0	29
Setting up a physical facility for industry or a spin-off company	100% 29	0% 0	0% 0	0% 0	0% 0	29
Other	71.4% 5	0% 0	0% 0	0% 0	28.6% 2	7



Question 12: In the last 3 years, how many different companies have you and your team worked with (i.e. had some sort of funding from)?

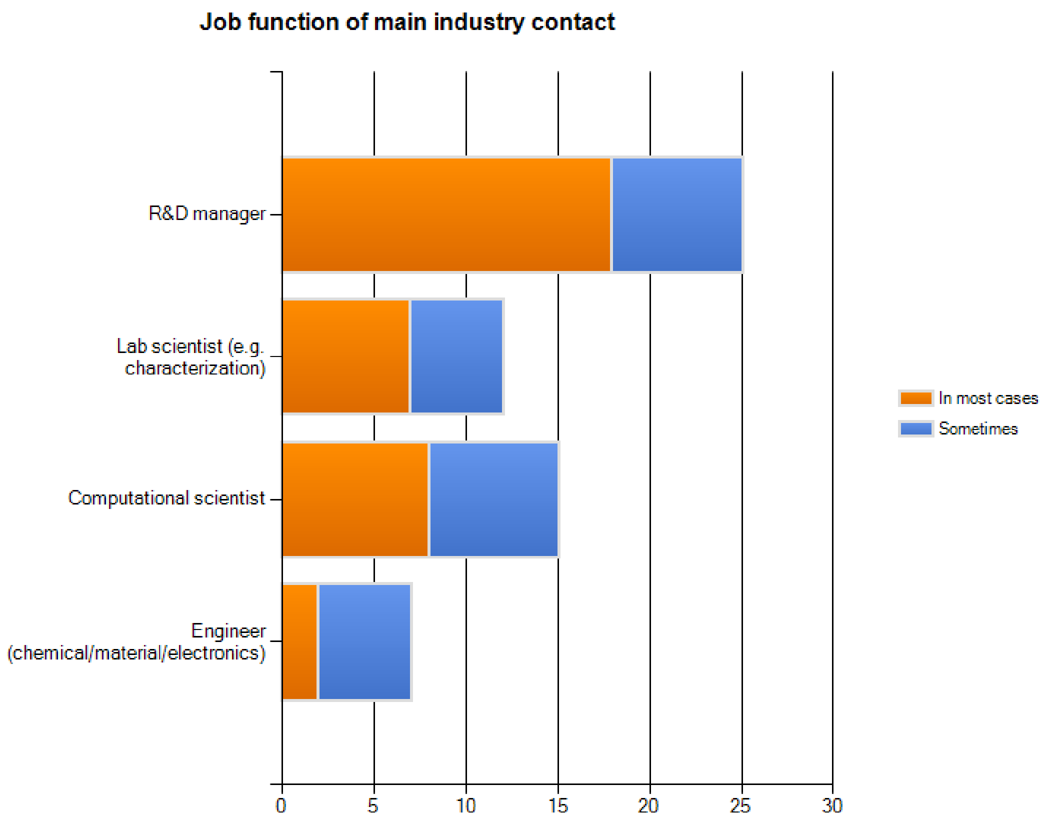
With government funding	Without government funding	Any type
30 responses	30 responses	30 responses
9 have no project	9 have no project	3 have none of either type
70% have projects with government funding	67% have projects with government funding	90% have industry collaboration
Average 2 companies	Average 1.4 companies	
Average excluding those without collaboration: 2.9	Average excluding those without collaboration: 2	
Maximum: 8	Maximum: 6	

Question 13: In the last 3 years, how many different industry funded projects of what different duration has your team been involved with?

26 responses with the following totals:

With government funding				Without government funding			
up to 3 weeks	3 weeks to 3 months	3 months to 1 year	Longer than 1 year	up to 3 weeks	3 weeks to 3 months	3 months to 1 year	Longer than 1 year
0	0	1	49	2	4	6	35

Question 14: What is the job function of your main contact in these industry projects?



Measures of success

Question 15: What is your longest standing industry collaboration?

Average: 73 months and Median: 48 months and maximum: 192 months

Question 16: How many renewals/projects have you had with the same company?

Average of 3, median of 2 and maximum 10

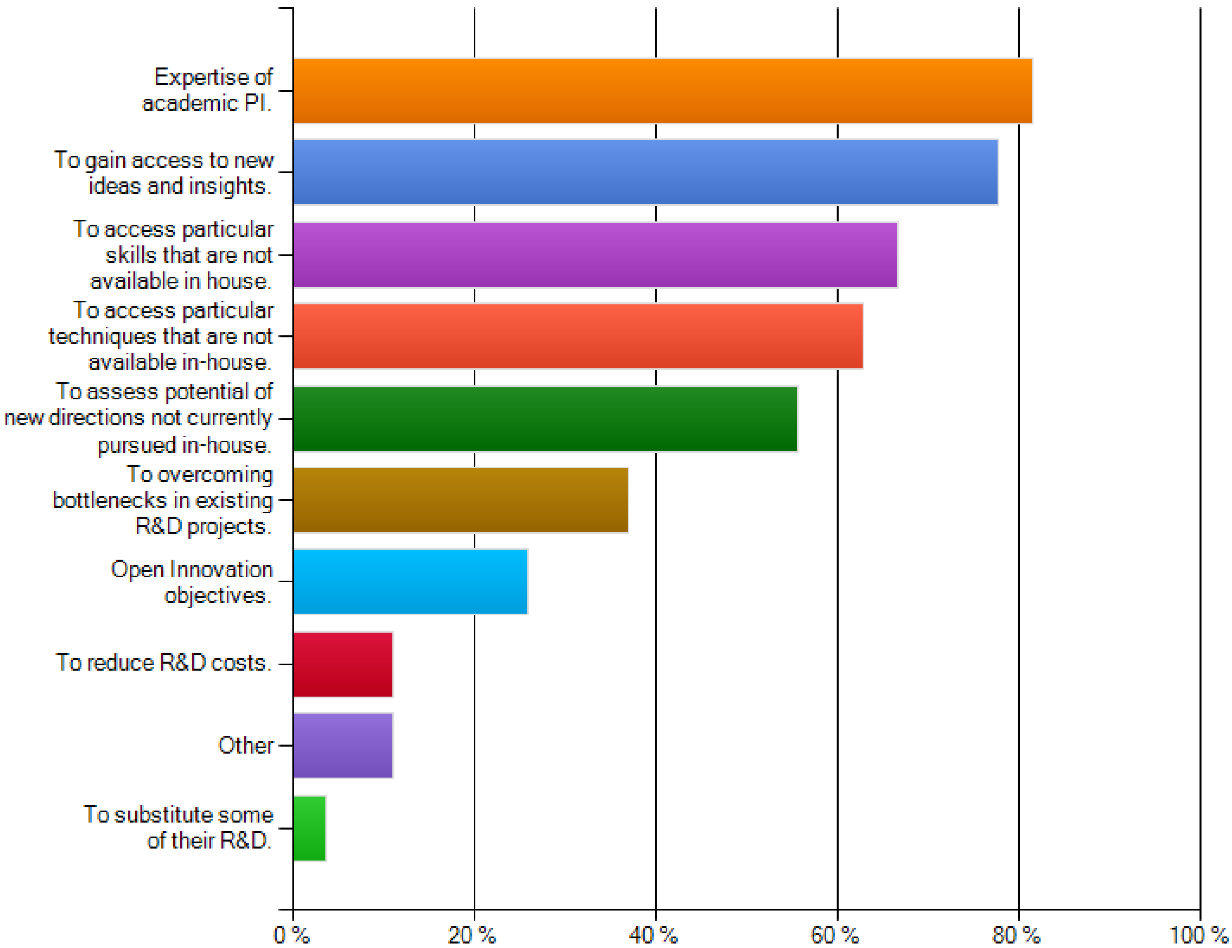
Question 17: How many companies do you collaborate with on average at a given time?

Average of 2 and maximum of 5

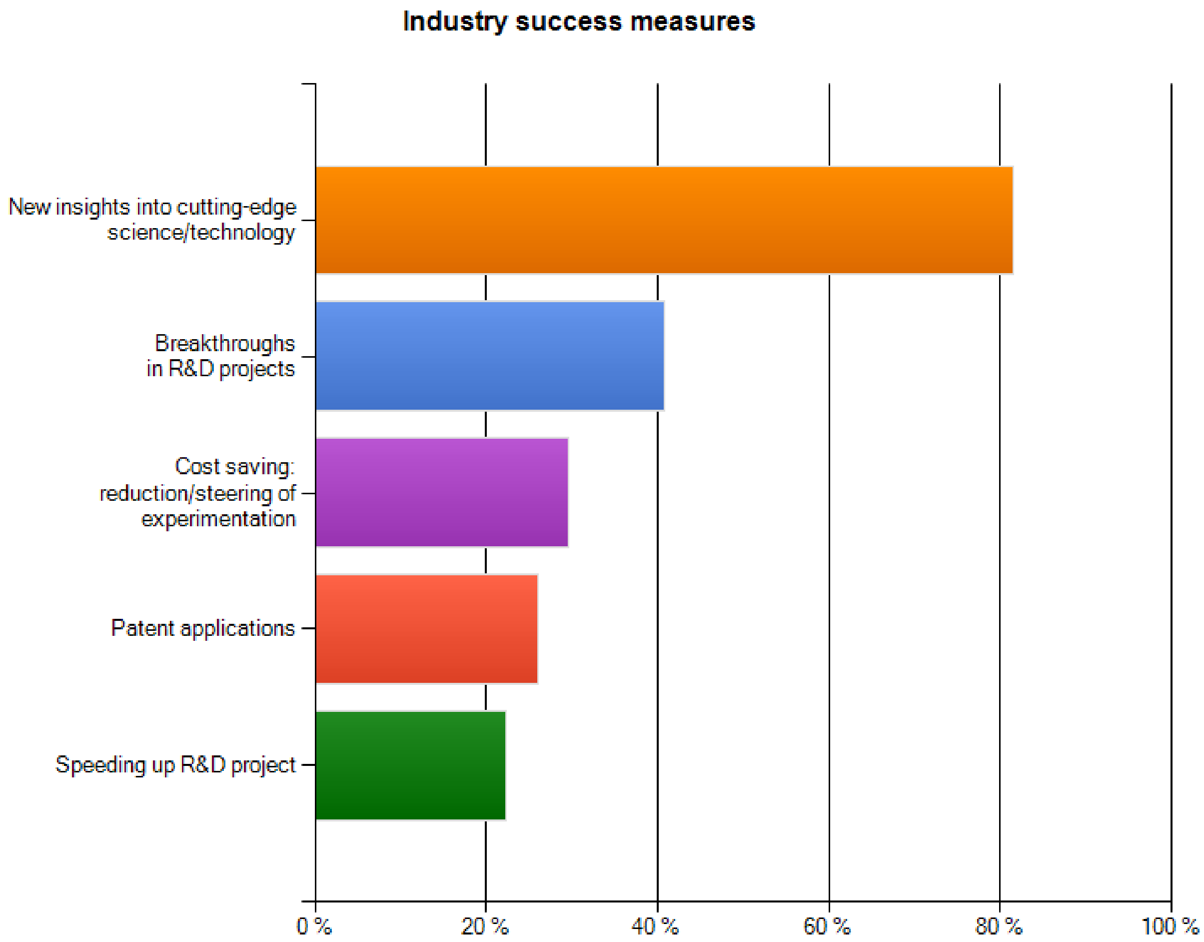
Question 18: What percentage of these companies are in Europe?

Average: 84%, Median and Mode: 100 %

Question 19: What are the main reasons for your industry collaborators to enter into projects?



Question 20: What measures of success are applied by companies?



Question 21: What have been the key success outcomes from your perspective?

- Publications: Since most of the industry interactions are research collaborations, publications are a key outcome, and most respondents noted several or many publications, including "high-impact publication with technological relevance".

- Patents: while patenting activity was not regarded as a major driver, a quarter of respondents nevertheless reported patenting activity resulting from industry collaborations.

- Royalties: about 10% of respondents reported royalty income from software development. See also the section on codes developed by the network, integration in commercial software packages and distribution into industry.

- New methods: about half of the respondents noted that new methods were developed as a result of the collaborations. In fact some of the responses noted that "new problem sets and driving capability is one of the main incentives", that these collaborations bring up questions that would not otherwise come up, and that "one of these methods has attracted more than 100 citations". In addition, a positive outcome has been gaining new ideas and perspectives from sharing of expertise with industrial research groups.

• Funding for research ranges from zero or quite small amounts to substantial amounts, i.e. millions of pounds/euros. About three quarter of respondents had students trained as a result of industry interactions.

Question 22: How many students have been trained in your group in the last 5 years that then went on to work in industrial R&D?

- Entered into computational roles: average 2 and max 6
- Other roles in industrial R&D: average 2 and max 10

Question 23: Please provide examples and success stories.

- Solidification in casting. Understanding of the free energy of the crystal in contact with the melt.
- Failure, plastic deformation and creep resistance in high T alloys. Mechanisms by which commonly trace elements work.
- Identification of deep/shallow donor and acceptor impurities or defects in spinel compounds.
- Unveiling of the conduction mechanisms in CNT filled polymer composites at low loading and elucidation of the mechanisms of conductivity in CNT filled polymer composites using a combination of codes including *ab initio*.
- High performance optical layers with tuned absorption and diffraction properties, achieved by computational screening. Modelling also helps with optimising the manufacturing conditions (using classical potential methods) by simulating the segregation/deposition.
- Ice formation and its inhibition on supercooled substrates.
- Failure mechanisms in high performance steels, which exhibit extreme stiffness but should still be ductile/formable and absorb energy on impact. Gain understanding via calculation of energetics of different mechanisms and different chemical constituents.
- Hydrogen embrittlement and failure. Very difficult to investigate experimentally, but with *ab initio* the different mechanisms and hypotheses can be investigated.
- Graphene functionalization
- Thin-film window coatings.
- Improved thermal stability of hard coating films via multicomponent alloying, leading to a patent application for coated cutting tool insert.

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