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Effective Industry−Academia Collaboration Driving Polymer Innovation

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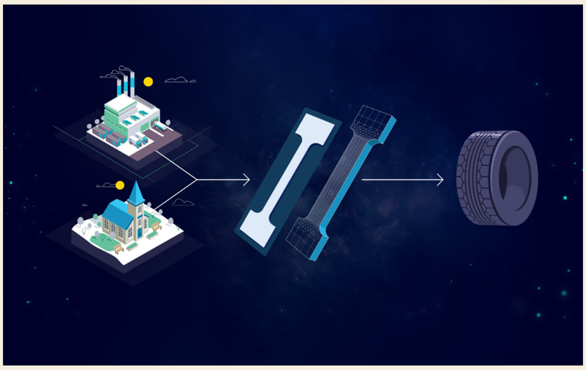
ABSTRACT: Polymer science is one of the few fundamental research fields where the results can be transferred into real-life products almost immediately. Industries need collaborations with the best researchers (universities or national laboratories) to elevate the field and favor the development of new materials, which will boost the chemical and materials business economy and ensure that innovative and sustainable polymer products are constantly being brought to the market. The mechanisms to ensure a seamless and fruitful collaboration are numerous, but few approaches really manage to incorporate the full range of polymer research from a molecular understanding to a macroscopic control of properties. We review some of the main components of standard industry−academia collaborations and propose to develop *polymer open centers* that put the business development objective as the starting point of the collaboration and allow those to gather and focus on different scientific fields toward a common objective.



KEYWORDS: *academia, industry, collaboration, polymers, digital*

1. INTRODUCTION

Effective collaboration is at the cornerstone of efficient research and innovation. Academia pushes the frontier of polymer science, and many industrial companies contribute to the polymer community. *"Academia" will be used in the text to encompass both university and national lab research*. Groups are collaborating through grants, exchanging and challenging their ideas in conferences, or inviting each other to seminars and workshops. The polymer community is active and well-structured, as confirmed by the number of polymer scientist organizations (APS division on polymers,[1] ACS division of polymer chemistry,[1] Softcomp,[2] Japan society of polymer science,[3] etc.). Compared to other scientific fields like strongly correlated electrons or cosmology, soft matter and polymers are unique scientific fields where the most fundamental research can be translated into an industrial application almost instantly. This is due to the ease of integration of new concepts directly into production without requiring significant additional infrastructure. This rapid application of fundamental research leads to vivid competition between industrial groups, which makes them constantly innovate and understand the scientific discoveries that could enhance the performance of their products. Moreover, to deploy these research topics within the industrial organization, they need to hire new talents with *updated* competencies, which requires companies to be scientifically attractive for the younger minds and to propose a career path that will quench their thirst for innovative but applicative research with a high capacity of growth.

Industrial groups may use different partnership models with universities, national laboratories, or startups to co-develop science and technology and gain access to the most recent research while interacting with students and postdoctoral fellows that could be interested in joining them. However, this process is not always as simple as one could imagine. Depending on the collaboration model used, sharing intellectual property (IP) can become a real puzzle for lawyers. For the company, it is not necessarily easy to share relevant industrial data to an academic partner when highly competitive topics are at stake. On the other hand, it is vital for the career of students and postdocs at the university to publish the work.

In section 2 of this perspective, we will review the main elements that need to be considered in order to develop an effective and efficient industry/academic collaboration in polymers. Section 3 will briefly present the most common models of collaboration that are currently used and discuss the

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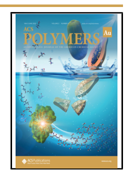

important question of IP. Section 4 will describe a proposal for more effective collaborations and some perspectives on how to move forward the development of scientific polymer discoveries with faster turnout into new products and new industrial innovations.

2. ADDED VALUE OF INDUSTRY−ACADEMIA COLLABORATION

Setting up a partnership between an industrial company and an academic institution can be complex at the contracting level, stressful at the IP level, and costly for modest industrial entities. In the case of "digital" polymer science (simulation, modeling, or artificial intelligence (AI)), this can become even more tricky as there is often no clear understanding in the community on what is IP when it comes to model, data, or simulation results. Companies that have no R&D department or a limited size one will still require innovation to boost their sales and satisfy their customers. Therefore, they embark into the endeavor and seek academic partners: the need outweighs the complexity of the industry−academia collaboration. However, why would a major industrial institution with thousands of employees in its R&D function decide to collaborate with an external entity? They already invested millions in their hiring process, even more in providing salary and incentives to their employees and significantly more in developing and maintaining their research centers and scientific equipment. However, to remain *up to date* in their field, attract new scientific talents, and sometimes reduce the cost of conducting their own research and development, they look to the academic world for the source of their own innovation. Additionally, some funding and resources are uniquely available to researchers at a subsidized/reduced cost. In 2010, Traitler et al.[4] expressed the importance of bringing together compatible differences to secure an efficient collaboration mechanism, and indeed, academic and industrial entities do not necessarily share the same desired outcome for their joint research. One is interested in the world class science that will be published and the other one in the applicability of the work toward new products or service for their customers. Strong partnerships in polymer science exist. BASF established a strategic research initiative called BASF's "Northeast Research Alliance" or NORA at Harvard.[5] De Pablo et al. and Solvay have worked together to build some new coarse-graining approaches for polymers.[6] Multimechanics, Inc. worked on crack propagation modeling with different universities.[7] Everaers from ENS Lyon has built some strong partnerships with Continental that bring together modeling, simulation, and experiments.[8,9] Ginzburg, from Dow, Inc., has developed ground-breaking polymer research throughout his industrial career.[10−12] Industry−academia partnerships should be a win−win collaboration to become successful. We believe that there are three main parameters that need to be considered to allow this:

1. an exchange of information between the best in class
2. a beneficial financial mechanism between institutions
3. a focus on the growth of future talents

2.1. Working with the Best in Class

Successful innovation partnerships based on open sharing of knowledge accelerate co-development of innovation.[13,14] The problems addressed during the collaboration need to be both scientifically relevant for the academic partner and impactful in the industrial business. For example, the work performed by Leo (Solvay) and Govaert (Eindhoven University of Technology) on embrittlement of polymer glasses has been carried out over many years because of its complexity and scientific relevance.[15−17] Couty (Michelin) and Malfreyt (CNRS, Université Clermont Auvergne) have worked on polymer and polymer nanocomposites over the last 10 years because it still remains a very active field of research.[18−21] At the experimental and synthesis level, it would take years to list all of the fruitful collaboration between universities, national laboratories, and industrial companies. The work of Piunova at IBM (now at Loliware) on biofouling protection, for example, is remarkable,[22,23] and the long-lasting collaborative work between Bates at the University of Minnesota and Dow, Inc. have been recognized by the ACS through the 2008 ACS Cooperative Research Award and many publications showcase the quality of this work.[24−26]

To ensure a successful partnership, the industry partner should not be shy in sharing relevant and up to date industrial problems and corresponding data. The academic partner will understand that when IP is at risk, these data are to be kept only between the two parties. When collaborating with the best in class in the academic world, the industrial partner must accept that the project should not be a simple execution of a simple problem or a repetition of a known method on a multitude of use cases. The work has to be unique and original enough to be published. The work has to be also mutually interesting. An industrial employee should not come and visit an academic partner prospect with a closely defined project. Instead, a list of long-term problems should be presented and allow for the academic collaborator to propose his/her own research path in accordance with his/her group research interests. It is not always easy for an industrial researcher to commit to a sustainable long-term research collaboration as industrial companies can sometimes change their objective at a time frame not compatible with a long research program. However, those long-term projects are the most valuable and can bring long-term value. It is the responsibility of the industrial researcher to translate the scientific discoveries into actionable tools and industrial applications.

In a nutshell, there is a clear added value for both entities to work on industrially and scientifically relevant problems. Each party needs to understand the interest of the other one to be able to build the trust that the partnership requires. For an industrial company, there is always a price to pay to work with the best in class: the best professors in the field are busy, they might not need the money to run their group, and therefore, they only work on a project that brings value at the scientific level. High impact factor scientific publications need to come out of the project. There is no need to connect with highly recognized academic professors to work on simple projects or direct applications of a known methodology as this is the role of the industrial scientists.

2.2. Financial Mechanism and R&D Investments

Understanding the stakes of academic and industrial entities is important before engaging into a contractual relationship. Most of industrial financed projects with a university will involve three kinds of costs: the student or postdoc salary, the supervising professor contribution, and the overhead (including administrative and sometimes materials/computation costs). Except for some very specific consulting cases, the professor contribution is usually negligible; the salary cost of the student or postdoc is likely to be comparable from one institution to another, but there is probably room for improvement to lower the barrier to entry by reducing the overheads costs. R&D is expensive, and long-term research is getting more complex to finance in corporations. It is more complex to justify an external expense if it becomes more expensive than hiring a full time employee in an industry sector that tends to reduce its workforce.[27] Leveraging on long-term relationships to allow a reduction of the overhead cost of industry−academia collaborations is probably a route to develop further to ensure a strong and sustainable partnership.

2.3. Attracting Talents and Preparing Them for Their Future Job

Long-term relationships favor a smooth transfer of talents from university to industry. When partnering with Ph.D. students or postdocs, a company can both train them and evaluate them. At the same time, the talents can evaluate the company they are interacting with and understand the difference between an academic career and an industrial R&D position. They get familiar with real industrial environment and problems. This can have a major differentiating impact when they look for a job—in their sponsoring company or any other.

By hiring these students and postdocs, companies are ensuring a simpler and faster integration of these new employees. More importantly, they ensure that new competencies and skills are constantly added to their research workforce. In the specific case of simulation, modeling, and data science in polymer research, there is still a cultural gap to breach to ensure a sustainable acceptation of these techniques into the R&D competency portfolio. There is therefore much pressure on the university to deliver results. This comes also with a higher chance to get a glowing career in the company if the collaboration is successful.

By interacting with top tier industrial companies, the student or postdoc working in the collaboration is easing his/her inclusion in the polymer community. If he/she decides to move toward an academic career, he/she initiates potential future collaborations which can help establish funding sources for future academic research or enabling successful future partnering with national laboratories.

Finally, interacting with talented individuals also pushes the rest of the company toward improving scientific excellence. Managing a collaboration on a high end scientific topic puts the industrial employee into constant challenge of his/her own knowledge and expertise and expands it.

2.4. A Win−Win Partnership

Starting an industry−academic project can be complex, expensive for the company, and difficult to manage at the contractual or IP level (section 3.2). However, the added value of the work outweighs the drawbacks. From a talent acquisition perspective to the capacity to develop first class science and innovation, the company can substantially benefit from the interaction and collaborative work, but the overall approach should also be seen as a unique opportunity for the academic partner. First of all, industrial problems are real scientific challenges. Major scientific papers have been cosigned by industrial and academic partners both at the *digital level*[6,10,28−33] and at the experimental one,[34−36] demonstrating the common interest and the relevance for the polymer community. These exchanges are also key to ensuring a sustainable economic future for the participating countries. When academic entities—in charge of teaching the talents of tomorrow—and industrial companies—supporting the economy through employment and growth—collaborate, they ensure a bright future by facilitating the development of new and innovative products while managing the renewal and development of competencies and skills for the workforce.

3. HOW IS IT DONE TODAY?

Multiple approaches can be taken to run an industry−academia collaboration: from a simple and closed *directed* research project to a more complex and open research center between multiple institutions. We will present in section 3.1 some of the most common ones and discuss in section 3.2 the important parameters to take into consideration when discussing industrial properties between an academic institution and an industrial company.

3.1. Different Models

The type of collaboration model should reflect the ambition and be commensurate with the complexity of the project. In Table 1 we present a non-exhaustive list of models used, their applicability, and the corresponding IP approach.

Among these models, the joint research center or laboratory is probably the less standard while being maybe one of the most productive. In this approach, a research consortium is created as a new legal entity controlled by more than one partner (company or academic). Laboratories get colocated within the industrial research building with the ambition to bring together researchers, students, postdoctoral fellows, engineers, and technicians into one single place of research. The CNRS (Centre National de la Recherche Scientifique) in France has been a precursor in this type of partnership.[37−39] By facilitating the exchanges between researchers for both institutions, these partnerships enhance the chances to develop breakthroughs[40−42] and promote the transfer of talents (and ideas) from one partner to another.

3.2. The Important Question of Protecting IP

Value creation is the main objective of industrial companies when financing R&D projects. The productivity of a project is measured by its capacity to transpose the research into products or services that will create business opportunities for the company. Patents are protected and even confidential for some time before being publicly published. For the academic partner, research is mostly evaluated by the scientific publications and communications that are published during a project. Papers are clearly public. It is therefore key to ensure a good balance between the protection of IP that the company needs and the objective to publish that the university seeks.

Our experience shows that it is always possible to publish on industry−academic collaborations. Even though it is likely that the company will require a preapproval of the publication before submission, it is generally easy to apply the new innovative technique or scientific discovery on a known polymer system use case. The contract written for the project collaboration should state the restrictions on publishing and define the level of control that the company wants to impose on the submission process. Establishing the contract represents usually the most complex part of the negotiation process. Recently, some academic institutions have been trying to impose more restrictive IP control: preventing the company to co-own the discovery of the research or imposing them to pay a prohibitive license fee to use the outcomes of a contract they financed. However, the scientific advances can be handled with the concept of "open science": patents and paper (in that order) are published at the end of the contract, and both parties can use the outcome of the collaborative research without further authorization. The

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Table 1. Different Standard Collaboration Models

model	deliverables	good for ?	IP
academic consulting	no specific deliverable	evaluation of research strategy	secured through an NDA
fellowship	no specific deliverable	first touch on a research topic; discovery research	cannot be secured
directed projects	specific and targeted deliverables and objectives	short- to medium-term research with well-established approach; application of known techniques on new topics	controlled through a contract
multiyear collaboration	the theme of research is defined; specific projects are signed throughout the collaboration to decide on specific research topic	long-term development	controlled through an umbrella agreement; specific IP issues can be renegotiated at the project level
university-centered industrial partnerships	multiple themes of research can be defined	long-term research	precompetitive projects to avoid IP blockade between companies
joint research center or laboratory	multiple themes of research can be defined; projects can span over many years	long-term partnership on advanced research topics	controlled through an umbrella agreement; specific IP issues can be renegotiated at the project level

company develops a new material that they can commercialize. The university pushes further the science that has been started within the collaboration.

When transforming the scientific discovery into a product development, the partnership contract usually proposes a remuneration mechanism for the university based on a percentage of the benefits the company achieves after commercialization. This is a fair retribution to the scientific efforts that originated the commercialization of the product, but these percentages are difficult to evaluate in reality because the cost of industrialization of the production, for which the university did not contribute, has to be carefully calculated to evaluate the profit that an invention has entailed. A few universities are therefore promoting the concept of "upfront payment of IP rights". Here, the idea is for the company to pay an extra percentage of the collaboration cost (of the order of 10−20%) to cover all IP and licensing costs moving forward. For the university, it is a way to secure some money, even if the collaboration does not conclude with a major commercial outcome. For the company, it is a way to prevent complex license and IP negotiation. We believe it is a wise approach that should be developed further.

3.3. What Is Missing?

The models presented on Table 1 are interesting for developing a common field of research (university-centered industrial partnerships or joint research center or laboratory) or for tackling a specific subpart of a larger industrial problem (directed projects or multiyear collaboration). However, they lack in the business overall objective: what is the company going to do to implement the outcomes of the research into a product or a service for its customers? The best polymer science project can help to identify trends in mechanical response, compare some products, or eliminate some gross outliers. It is rarely expected that a 1 year research project can unblock the newest innovative product. Therefore, the author believes that a different approach is needed to result in the true potential of industry−academic collaboration: a polymer open center (see section 4).

4. WHAT'S NEXT?

In this section we will propose a different approach of industry−academia collaboration based on the context of *polymer open centers*. We will then describe how automation and data science (AI and machine learning (ML), in particular) are the logical and necessary components of a successful polymer-based industry−academia collaboration (section 4.1.3). Finally, we will develop this concept for an important industrial problem in section 4.2: nanocomposite materials for tire application.

4.1. Polymer Open Centers

Industrial problems are very complex. Not only are the relevant physics and chemistry happening *far from ideality* but they also require different scientific competencies to be understood. As an example, the mechanical behavior of a filled elastomer used in a tire is influenced—among other things—by the solicitations of the road, the abilities of the driver, or the air pressure inside the inner liner. It is also fundamentally controlled by the details of the chemistry of the polymer used and the interactions between this polymer and the filler.[43−45] Understanding the details of such a problem requires therefore scientific knowledge in many fields and cannot be addressed by a single academic laboratory. We believe that industrial companies could be the missing link by leading *open research centers*, using the same approach NSF or

DOE would develop, with the purpose of bringing together researchers from different fields of science toward the same large and ambitious goal. In this context, the collaboration would be solely based on the project objective. Such research centers would be *open* and *temporary*:

- Open: instead of having one partner only, the company would leverage the competencies that can be brought from the "best in class". There would not be a need to share a common space 100% of the time, but this should be favored on a regular basis to maximize the possibility of interaction. For a specific industrial problem and to move forward in the development of solutions, the partner list could evolve with time. In a first phase, more fundamental research could be promoted, when in a second phase, engineering specialists could take the lead to favor a seamless development of the original ideas into a commercial product. A closed loop might be beneficial in case adjustments need to be made in the fundamental research or new knowledge gaps that come up during development.
- Temporary: When the project is over, the center would end as it is the project objective that solely justify the collaboration.

4.1.1. How Would It Work? The key element to start such a center on the industrial side is the project. What do you want to solve? What is the problem? How would solving the problem would bring value to the company? What would be the return on investment (ROI)? What is the relevant market? What share of market could I get if I solve the problem? When these business-related questions are answered and the need to move forward in a specific industrial direction has been justified at the upper management level, funding the project is easy. Too often has the author been frustrated by the complexity to finance a very good project because the management did not see the added value. We therefore recommend to start by evaluating this value.

In the same way a standard government-funded grant would operate, the proposed approach to start an open center is for the company to publish publicly a funding opportunity announcement (FOA) that states the needs and objectives of the project and describes the industrial problems to be solved. If the problem involves more than one company, the FOA would be cosigned, for example, to develop a part that involves a manufacturer and its provider. It also encloses the available budgets, the requirements to be part of the grant (export control, diversity, sustainability, cost share contribution if any, etc.), and the expected duration. If confidentiality is a major hurdle of the project, the company can prefer to directly contact the teams that could be interested in the topic and avoid a public disclosure of the project. However, these projects should be considered as long-term and fundamental to justify the effort, so the author believes that most of the research performed by the academic partners should be open for publication and therefore partially public. Starting a center openly through a FOA plays another important role: it emulates competition between research teams and therefore increases the probability to get the best in class to solve the industrial issue.

The interaction between the parties is key to ensure a fruitful collaboration and a transfer of the developed science into industrial products. Sharing a common place can facilitate these exchanges, and the approach described in section 3.1 for the joint research laboratory could be applied to the open center. Nevertheless, it would particularly challenging and expansive to impose a relocation to a list of collaborators for some years and would drastically increase the budget of the effort. The author therefore believes that the open center should remain mostly virtual and simply have a *common space* in the industrial environment. This would be a place for the members to visit on a regular basis, organize interteam discussions, or participate to project milestone meetings. Locating the space within the industrial environment bears a two-fold advantage: (1) the academic partners can obtain a concrete understanding of the impact of their research and gather direct information or experimental data points on their research; (2) as described in section 2.3, the students and postdocs get to know the industrial world they could join, and the industrial partner gets to know and evaluate their potential future talents.

4.1.2. Why Are Polymer Open Centers Different ? Compared to university-centered industrial partnerships (see Table 1), open centers are fully industrially driven and project objective centered. The company wants to solve one, sometimes two, industrial issue(s) and—in ideal cases—foster innovation toward new products sold to its customers. As in university-centered industrial partnerships, fundamental science is developed in an open center. Indeed, the most applied industrial problem needs sometimes the most advanced research. Understanding new science is therefore not to be done as the principal objective but as a means to solve the center problem(s). For example, when trying to create better polymer composites for weight reduction in the automotive industry, the fundamental understanding or polymer/fiber interactions will probably be needed to move forward in the market, but if this understanding is not needed to improve the product, it does not need to be achieved.

IP is obviously an important topic in such an organization. The grant contract should define the IP and license rights for all parties. As explained in section 3.2, the author believes that the upfront payment of IP licensing right is a preferable way to handle this question in a mutually beneficial manner. Compared to university-centered industrial partnerships, the industrial objectives of an open center drive IP terms toward a more controlled approach of publications. As discussed in section 3.2, it is often possible to apply new innovative techniques or scientific discoveries on a known use case to ease the approval of a publication.

4.1.3. On the Use of Automation and Data Science in Open Centers. With the rapid development of the use of data science, ML and AI for polymer research,[46] we believe that those centers should be "database-driven" and experimentally "high-throughput based" to generate data through modeling, simulation, and experiments and develop a toolbox for generating in silico-controlled systems before experimental implementation. Aubus et al.[47] nicely reported the importance of data collection and analytics in polymer science, and the improvement of *natural language processing* and *semantic* techniques should contribute to facilitate the automatic ingestion of historic science and data from publication and patents which will help the centers to perform more efficiently.

Additionally, high-throughput and automation techniques are becoming more common in the chemical industry. Startups like Kebotix[48] are combining cloud technologies, artificial intelligence, chemical informatics, physical modeling, and lab automation. This helps both to use modeling and experiments to create composite data set (both experimental and digital) for AI training and feed back the experimental setup automatically to speed up the convergence of the experimentation toward the

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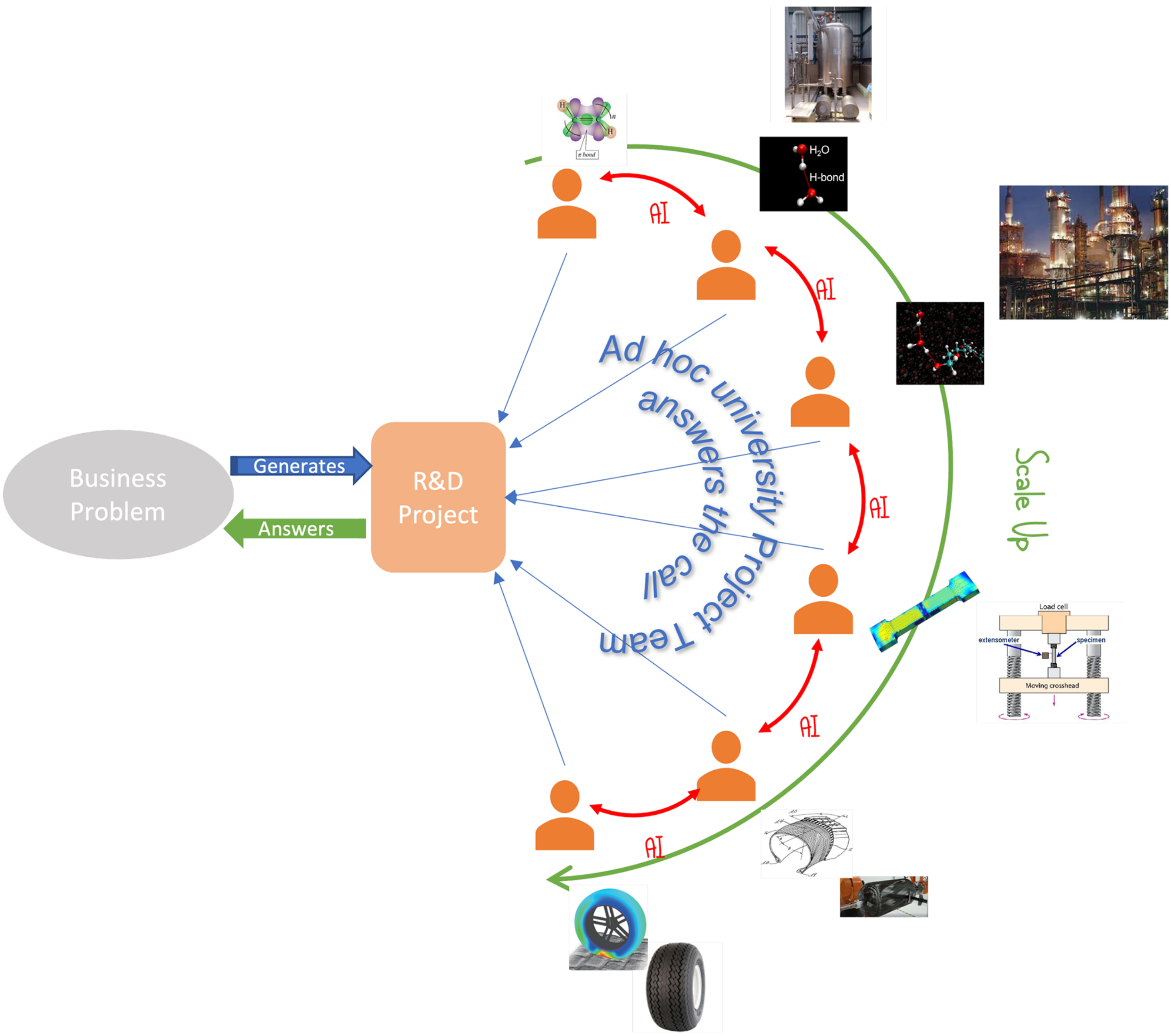

Figure 1. Polymer open centers.

best material for the desired properties. This approach should be at the cornerstone of the polymer open centers.

Finally, data analytics techniques can help to overcome the complexity of model order reduction and multiscale modeling. Molecular dynamics force fields can now be *learned* using machine learning,[49] allowing a scaling up approach from the quantum level to the classical description. At the other size of the scale spectrum, neural networks are now commonly used to accelerate mesh generation in computational fluid dynamics[50] or to create surrogate models for engineering problems.[51] We argue that data science will help to create seamless integration of digital and experimental scientific discoveries and fuel the open centers toward a resolution of the industrial polymer project.

A schematic representation of the mechanisms of a polymer open center is depicted on Figure 1.

4.1.4. Why Is It Not Done Today? The open center approach seems to satisfy a lot of the requirements for a profitable collaboration, but it is not widely used. Large companies's associated foundations regularly open FOAs associated with their charity or sustainability goals.[52−54] To the best of our knowledge, opening a massive scientific grant opportunity at a company-wide level is not done in polymer companies.

These ideas would represent large investments (see estimation in section 4.2), and it is probably the main barrier to entry. We argue that only a clear ROI evaluation and business plan can justify this level of investment. The predefined research budget publicly communicated within the FOA ensures a control of the expense. The predefined objective of the center ensures alignment of the research strategy between the entities involved. Moreover, we propose to leverage a public/private partnership to ease the financial complexity, but this should not be a prerequisite. This contribution should only finance the fundamental part of the center's research. As the objectives of such projects would impact the economies of the country where they would be created by developing science and innovation and new products and increasing employment, we believe that such a partnership can easily be justified and receive funding. The "industrial FOA" would clearly state the IP conditions, and

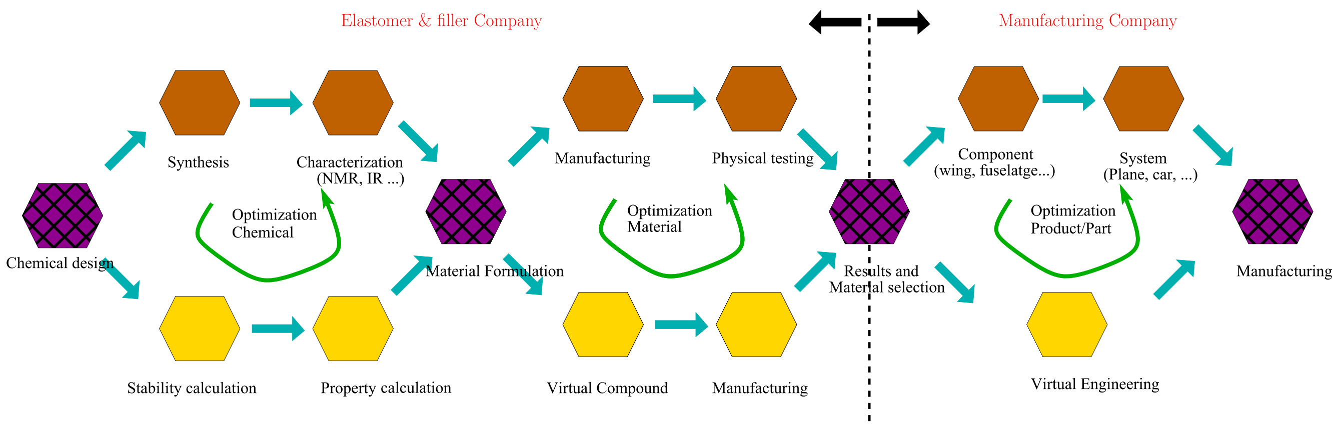

Figure 2. Complex route from the molecule to the part.

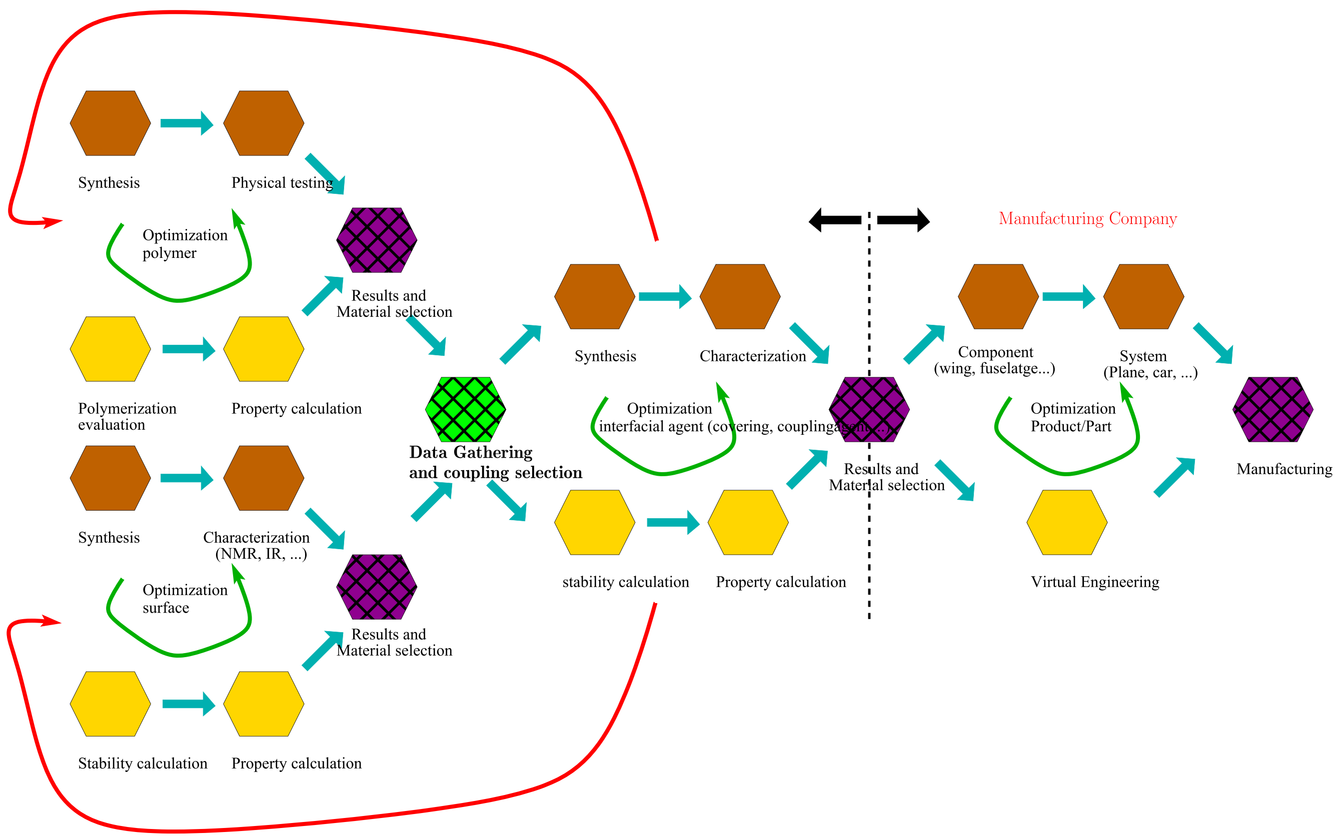

Figure 3. Important role of the interface design.

therefore, only universities or government laboratories agreeing with these conditions should apply.

4.2. A Relevant Example: Multiscale Modeling of Polymer Nanocomposites for Tire Applications

Let us consider the example of a polymer nanocomposite used for tire applications. For the sake of the example, we can focus on the tire tread. The (very) schematic representation of a new formulation development is represented in Figure 2. The objective is to link the formulation details to the final property of the part of the tire to be designed.

The type of polymer (elastomer in this case), the nature and concentration of the fillers (silica or carbon black), the chemistry of the coupling and covering agents (if any), and the procedure used to both synthesize/process the material and design and manufacture the tire part need to be optimized. The mechanical properties along with the failure (wear, fracture, etc.) properties are considered. Figure 2 shows the two "standard" routes that should be used in parallel to perform this optimization. At the top, in brown, is the experimental part, and at the bottom, in gold, is the in silico route. The left part of the graph is the realm of the materials company, and the right part is the domain of the car manufacturing company. The connection is done at the material selection level, where the properties required for the manufacturer are requested from the material company. In some cases, the material and manufacturing companies are the same.

One extra level of complexity comes here for the complex interaction between the polymer, the filler, and the potential covering/coupling agents used when silica is chosen as the filler (traditionally silanes). Not only should the polymer be designed

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but also should the chemistry of the nanoparticle surface, their sizes, and the chemistry of the silane if any. A better representation of the design process is therefore represented on Figure 3.

This is a typical example where the approach of a *polymer open center* would be beneficial for an accelerated design of a tire tread. In this example, a joint FOA published by both material and manufacturing companies to gather the best in class could be envisioned. At the "digital" level, options already exist to tackle part of the left or the right of Figure 2. Schroedinger,[55] Biovia Material Studio,[56] Culgi,[57] or Scienomics,[58] for example, propose materials platforms that can calculate the properties of materials or chemicals ahead of synthesis or characterization. Some of those software editors leverage ML to optimize the chemicals according to a set of properties. Similarly, material property can be evaluated, predicted, and optimized using platforms such as Siemens Simcenter Multimech,[59] e-xstream Digimat,[60] or Ansys Mechanical,[61] with the common trend to develop AI or ML tools to perform the optimization. Most of the tire companies have developed their own tools to deal with large-scale modeling.

At the experimental level, tire companies have a large expertise in the synthesis of elastomers, the mixing processes, and the molding/curing of tires. Their industrial setup is strong and mature and, for the most part, optimized. However, the interplay between materials chemistry and final properties of the tire is not fully integrated. Some efforts are made to bring the different scales of polymer science together. Experimentally, silica-producing companies partner with elastomers/tire companies to speed up innovation.[62,63] Other tire companies have started joint laboratories with universities or government laboratories.[64,65] Numerically, Siemens Simcenter or Dassault 3DS propose a software portfolio that can span the entire time and length scales of Figure 2, but the integration is still not finalized. There is therefore room for industry−academia collaboration that would span a larger objective: for the molecule to the part. For a problem like the optimization of materials in a tire, the final part properties, the sustainability of the material, and the objective of light-weighting call for an efficient connection between the chemical synthesis of the materials, its optimization, and the design of the final part. The connection between scales is heavily problem-dependent, both at the experimental and the digital level. The scientists in the different fields to be involved do not sometimes speak the same language. The *strength* of a material can be described by the cohesive energy, the Young's modulus, the yield stress, the maximum shear stress, etc., depending if you are a quantum chemist, a physicist, a material scientist, or a design engineer. The author therefore argues that gathering the above-mentioned professionals within the same center and ensuring that they focus on the same project objective through constant communication would represent an important upgrade moving forward (see section 4.3).

Starting such a center would have a significant cost. To span all of the scales and address all of the questions, one would need to gather for ≃4 years a combination of 6−8 scientists (Ph.D. students, postdocs, professors, engineers) at the digital level and 6−8 scientists at the experimental level. Adding materials, equipment, and building location, we can evaluate a need of ≃ $20 million investment. However, the scientific platform resulting from this center would easily be expanded to any other part of the tire or of future tire designs. It would also *by construction* include the fabrication/manufacturing requirements along with the feasibility of materials production.

The development of an industrially led open research center of this kind would represent a concrete realization of a full integrated computational materials engineering[66] and a key milestone in the realization of a true *digital twin*[67] of the production of car parts made of a polymer nanocomposite. It would speed up the development of prototypes and the transfer from prototype to production, significantly impacting the cost of new tire development.

4.3. Shared Advantages of Polymer Open Centers

An open center in polymer science can bring value to all parties.

- Academically:
  - Accessing the industrial data seamlessly allows one to use it when developing new experiments and/or new models.
  - Ensuring a collection of both experimental and modeling/simulation data when developing the materials and improving the design will dramatically enhance the capacity to develop executable AI models
  - Developing the AI connectors to allow a systematic model order reduction from the smallest scales to the largest ones will contribute to a more efficient multiscale modeling of polymer.
- Industrially:
  - Developing an AI-based platform to better design the part while choosing the most appropriate material would be an asset. By collaborating through the open center, both the material and manufacturing companies are working on a project that should generate major revenues.
  - Establishing the appropriate network of academic and industrial experts through the center will allow for an extension of the platform to more products.
  - Defining in advance the IP rules of the partnership will facilitate an open exchange between the partners ensuring that the platform is *spot on* in developing the appropriate science for the problem at stake.

5. CONCLUSIONS

Effective industry−academia collaboration can drive polymer innovation by leveraging on the best in class of both worlds. To propose to their customers new innovative materials and material parts, both chemical companies and manufacturers need to boost their innovation thanks to relevant collaborations. Polymers account for more than 500 billion dollars in products. The growth rate for this business is supposed to double the U.S. GDP[68] growth rate. We propose that *polymer open centers* can drastically speed up the development of new products by focusing on a common industrial business goals and entail a bright future for this industry.

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Notes

The views expressed are those of the author and do not reflect the official policy or position of Siemens. Some examples of successful industrial−academic partnerships in polymer science are described in the documents; those are just a small sample out of many that the author could have chosen.
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