Advice for Emerging Researchers on Research Program Development: A Personal Case Study

Christopher W. Jones

School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA 30332-0100

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Introduction

ach year, hundreds of new scientists and engineers start their independent research programs at universities, government laboratories or other institutions. Every individual embarks on this pathway with some idea about what research directions they wish to undertake, but often, with little insight into how their research career may evolve over time. Furthermore, there are relatively few descriptions of how the research programs of other scientists and engineers have developed over time. In most cases where such overviews are available, they are written towards the end of a researcher's career, at a point far from the early development of the program. In this work, I provide my personal thoughts and observations on the development and evolution of the first 16 years of my research program as a case study. This overview does not intend to suggest this particular case as an exemplar, but rather, provides a single example of how one program evolved. In the course of the description, I try to identify general observations and suggestions that might aid a new researcher in the chemical sciences or engineering in the development of their research program. In particular, the focus is on a program where the newly independent investigator has significant autonomy to select research topics of her/his choice (e.g., many universities, some government or corporate labs), although it is recognized that in many organizations, a researcher must fit into and adapt to the specific needs of the host institution.

A particular aspect of my research program is that it blends research on (1) materials chemistry, (2) catalysis and reaction engineering, and (3) separations. As such, I will draw from specific examples of my own work in these fields as part of the discussion. However, the reader should note that this perspective is not a traditional overview of the full breadth of the title research topic, although my group has written such reviews and perspectives on a variety of the subjects covered here.^{1–6} Instead, here I discuss how my program evolved in stages, including (1) the search for a position, (2) launching your laboratory, (3) development of research themes and finishing with (4) a summary of advice for researchers starting their independent laboratories.

The Search for a Position

Developing a compelling theme for a new research laboratory is one of the biggest challenges an emerging researcher will face. The natural inclination is to most often propose an extension of one's own thesis work. However, in many institutions, this can be viewed as too incremental. As such, it is critical that an aspiring independent researcher spend a significant amount of time and energy developing new research ideas, ideally in a continuous, iterative fashion. This can best be done in conjunction with trusted advisors. Often, initial ideas are not well-thought-out, or are derivative of past work, and iteration of ideas with more experienced researchers can help an aspiring principal investigator (PI) identify research topics that will define a niche, or brand, for which the PI can establish a unique and visible research program. In my experience, this research project formulation phase, whereby ideas are formally described in a written proposal or oral presentation, should start 6-9 months before application for an independent research position. Often, a period of ideation and revision can last for several months, followed by integration of individual projects/ideas into a cohesive and distinctive research theme. Starting this process early is extremely beneficial.

A key way to develop a unique combination of knowledge and experience that will enable creation of a distinctive research program is to choose a postdoctoral experience (or two!) which, when combined with the experience gained in the PhD, enables the researcher to attack new problems, existing problems in new ways, or both. But the choice of an appropriate laboratory for a postdoctoral position should not focus solely on the science to be learned and the research to be done; one should also consider other factors, such as the

Correspondence concerning this article should be addressed to C. W. Jones at cjones@chbe.gatech.edu.

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discipline of the laboratory (e.g., chemistry, biology, physics, medicine, chemical/mechanical/environmental engineering), the culture of the laboratory (e.g., large/small, collaborative or filled with researchers working independently, attacking fundamental or applied problems, hands-on vs. hands-off advisor, etc.). In addition to learning new technical skills, the postdoctoral stay is important for learning alternate student advising methods, group management skills and other critically important soft skills that most researchers are not formally taught, but are learned by watching others and experiencing different research cultures. The more research experiences an aspiring PI has, the more s/he has from which to draw in formulating their own plans.

When preparing to start the search for a position, there are several suggestions that may be helpful, based on my experience.

Be introspective

A key starting point is to make sure you know yourself, including your strengths and weaknesses. An introspective analysis will allow you to understand what specific attributes, skills or abilities you bring to a research program. In the context of catalysis and reaction engineering, it could be catalyst synthesis, kinetics, analysis of reaction mechanisms, specific characterization techniques, key computational methods, and so forth. However, this technical assessment is not the only aspect of self-analysis; perhaps even more important are your specific personality traits. Regarding your personal skills and work style, are you detail oriented or more interested in the big picture? Are you likely to wish to work on one or a few topics for an extended period of time, or do your prefer to explore new topics more often? To best position your research program for success, you need to know yourself, and how to position yourself to do work that moves science and technology forward.

Start preparing early. Define a unique theme for your program

Having an idea about what motivates you as a person and researcher, you next must identify a unique theme for your research program. A useful way to think about this is to develop a personal "brand" that you hope will one day be known and understood by your field. Examples from the field of catalysis include the Boudart/Iglesia and Norskov approaches to research. Michel Boudart^{7,8} (Princeton, UC Berkeley, Stanford) is known for pioneering an approach to heterogeneous catalysis research focusing on identification of the active site(s) in complex heterogeneous materials, estimating their number, identifying elementary steps in catalytic reactions, and characterizing catalytic performance using rates expressed as turnover frequencies (TOFs). This tradition has been continued and further developed by Enrique Iglesia9,10 (ExxonMobil, UC Berkeley), and today a significant fraction of catalysis researchers around the world carry out research following these principles. Jens Norskov (Technical University of Denmark, Stanford) has advanced the use of electronic structure theory coupled with linear free energy relationships to screen the reactivity of catalytic materials.¹¹⁻¹⁴ Density functional theory (DFT) calculations have enabled practically accurate calculation of thermodynamic and kinetic properties of elementary steps at active sites, providing an atomic-scale perspective on the surface phenomena and free energy landscape that underlies heterogeneous catalysis. This led to the important finding that the energetics of various surface processes are correlated with surface reactivity. Exploiting these energetic correlations in conjunction with microkinetic models has enabled the development of a quantitative and predictive theory that is now routinely used to screen and discover novel catalytic materials.

While one cannot establish a brand such as the two above before working in a field for an extended period of time, one can, even at the earliest stages, try to envision what their research brand might be. At the start of an independent research career, a research theme or brand is often more narrowly focused on a few specific research themes, either topically (e.g., polymerization, emissions control catalysis, methane activation) or based on techniques (*in situ*/operando characterization, etc.). In this task, it is critical that you leverage your personal expertise, while deviating in some key way from your past work. Generally speaking, if you are viewed as proposing to offer an incremental advance on your past work, or that of your thesis and/or postdoctoral advisors, it will be challenging to find a top position and become established as an independent scientist.

Timing is also critically important to finding a position and establishing a new laboratory.¹⁵ All research topics go through natural cycles of growth and decline, and it can be challenging for an emerging researcher to understand or predict these trends. For this reason, iteration of research ideas and topical areas with more established research mentors is helpful in shaping potential research themes (see above). In a specific example of poor timing, a major element in my research proposal while searching for university positions was to develop a molecular level understanding of how catalyst structure affects polymerization performance using supported single-site organometallic polymerization catalysts. As discussed below, not long after my laboratory was launched, interest in single-site polymerization catalysts waned at funding agencies and in the scientific community, meaning this topic never fully emerged as a research theme in my program. This leads to a key attribute that any successful independent researcher also must have, the ability to adapt, which will be discussed and emphasized further below.

A small but important element that an emerging researcher must address in their search is a knowledge of how their proposed research might be funded. To this end, some basic knowledge of how academic funding programs select research proposals for funding is worthwhile, along with what topics fall within the scope of the various agencies, foundations and corporations with which you might partner. A good way to gain experience in this area is by cowriting and coreviewing proposals with a senior mentor, allowing for discussions of proposal writing strategies, proposal strengths/weaknesses, and targeting specific funding agencies or organizations to be broached in the context of specific examples. For positions in government laboratories or industry, networking with scientists and engineers who are already working in such fields can help one learn how research is funded within these organizations. Such networking should be done before the job search begins. In most cases, a detailed plan to fund one's work is not needed, but a credible, hypothetical plan is desired.

Finally, in shaping your ideas and in writing descriptions of your proposed research, to the extent possible, always try to work on *the* problem rather than *a* problem. There are many good research problems in all research fields. The development of technical solutions to such problems will, of course, advance the progress of science and engineering. However, few problems are the problem, the topic/issue/challenge/question that most defines or limits the field. What fundamental knowledge would most enable a scientific breakthrough? What single problem, if solved, would lead to the most compelling advance in technology? The ability to define such a problem (the problem) will enable a researcher to position herself/himself for lasting impact in a field. In my experience, few researchers work on such problems early in their careers because they are both difficult to define and difficult to attack. In my case, after 15+ years of independent research, I feel I am only now becoming comfortable defining some of the most critical problems in my fields of research. Furthermore, some of the best problems, once defined, are extraordinarily hard to tackle with testable hypotheses using available research tools. Nonetheless, to the extent possible, identifying and addressing the most pressing problems in the field is the way emerging (in fact, all) researchers can establish themselves in a field and push the broader scientific enterprise forward. Even if defining or working on such problems feels daunting, if you can frame your research proposals as addressing topics that might be the problem in a field, rather than simply *a* problem, you are more likely to be a successful research fundraiser.

Launching Your Laboratory

In 1998–1999, I proposed to launch my independent research program studying the molecular design of oxide surfaces for catalysis, with an emphasis on polymerization catalysis. Having completed a PhD studying zeolites and other silica-based materials functionalized with organosilanes for applications in catalysis,¹⁶ I had a foundation of synthetic materials chemistry, heterogeneous catalysis¹⁷ and zeolites^{18,19} on which to build a program. During my studies, I developed an interest in supported molecular catalysts, but as an engineer, was troubled by the fact that they were not widely used due to stability issues.²⁰ I pursued a postdoctoral position in organometallic chemistry where I learned molecular inorganic chemistry and olefin polymerization catalysis. My goal was to study supported single-site olefin polymerization catalysts, which were successful examples of commercially viable supported molecular catalysts, as the initial focus of my independent research program. This topic was a good fit for me because (1) it was a topic in which my PhD advisor and his myriad former students in academia had not engaged, (2) it fit my technical interests and merged by PhD and postdoctoral training in a unique way, and (3) there were few others in my field (chemical engineering in the USA) who were studying this topic. To that end, after completing my postdoctoral year, I entered Georgia Tech as an assistant professor in the summer of 2000.

Go in with a plan. But be ready to deviate

I launched my laboratory with my first two students studying supported metal complexes as polymerization catalysts. Both projects involved the design and synthesis of supported transition metal coordination complexes tethered to silica supports, with one focused on single-use, coordination-insertion catalysts for olefin polymerization,^{21,22} and the other targeting recyclable atom transfer radical polymerization (ATRP) catalysts.^{23,24} Early in my term as an assistant professor, however, I began deviating from this initial plan.

While I was able to support both of these initial research directions with NSF funded projects, including a CAREER grant, the interest in the global academic community in olefin polymerization catalysis, which had been a dominant theme in organometallic chemistry for over a decade, began to wane. Recalling the advice detailed above, about knowing your own inclinations as a researcher, I also knew that I would be most happy and fulfilled if I was able to tackle an array of different projects. To this end, I sought to expand on my initial focus on supported polymerization catalysts.

One of my colleagues at Georgia Tech, F. Joseph Schork, had decades of expertise in radical polymerizations in dispersed media such as emulsions and miniemulsions.²⁵ Based on his interest in using controlled radical polymerization techniques in such media, and my group's experience in ATRP, we teamed to study reversible addition fragmentation chain transfer (RAFT) polymerization in miniemulsions. This fruitful collaboration went on for a number of years and several PhD theses,^{26–28} and is a good example of adapting to the opportunities that your home institution provides. Researchers working on a variety of topics in your organization may stimulate you to collaborate and take on new research themes. If you embrace these opportunities, you can more quickly expand your group and, therefore, your critical mass of researchers. I believe there are great advantages that come with a sizable group, which can provide enough researchers to provide a highly stimulating environment for everyone involved, including the PI, students and postdoctoral researchers alike.

Another opportunity that arose in my first year as an assistant professor was to partner and collaborate closely with another new professor, Marcus Weck,²⁹ who took an appointment in the School of Chemistry and Biochemistry. His group's expertise was in synthetic polymer and supramolecular chemistry, and the close alignment of our two groups, including weekly joint group meetings, allowed my group to rapidly improve its knowledge of polymer chemistry while also exposing Weck's group to our emphasis on catalysis and chemical engineering. Weck also had an interest in supported molecular catalysts, and in 2003, we teamed to launch a significant Department of Energy (DOE) funded collaboration that still continues today. In this project, we combined with three other PIs (3 experimentalists, 2 theorists) to explore the design of supported transition metal complexes used in important reactions in organic synthesis. This included carbon-carbon coupling reactions (Heck, Suzuki, etc.) catalyzed by supported Pd pincer complexes^{30,31} and enantioselective Co salen catalyzed epoxide ring-opening reactions.^{32,33} By the third year of my group's development, we had three key externally funded themes, (1) molecular design of supported single-site olefin polymerization catalysts, (2) controlled radical polymerization (RAFT, ATRP), and (3) polymer and silica supported metal complexes in organic synthesis. Only the first was part of my original plan, with the latter two directions stemming from

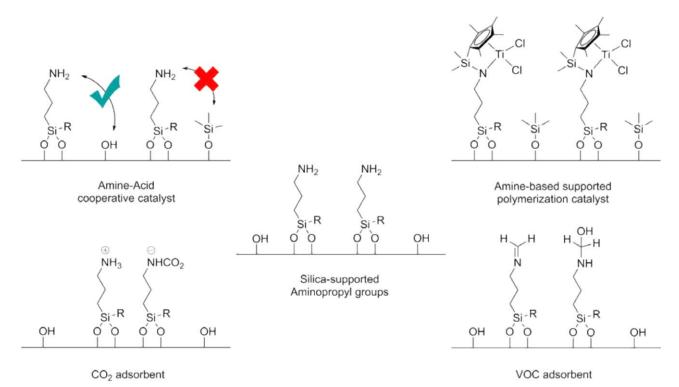


Figure 1. Silica-supported aminopropyl species (center) utilized in group's first two projects served as a launching point for an array of uses of silica-supported amines ranging from supported organometallic polymerization catalysts (top right), cooperative amine/acid catalysts for aldol and related reactions (top left), carbon dioxide sorption and separation (bottom left) and formaldehyde sorption (bottom left).

specific opportunities created by collaboration with other experts in my institution.

Embrace opportunities that present themselves

The programs discussed above all fit within the broad theme of catalysis and reaction engineering, and thus are consistent with how I viewed myself as a researcher when I started my independent career. Indeed, since my early days in research as an undergraduate student, I was always drawn to these aspects of chemical engineering, and this was how I saw myself as a scientist and engineer—as a catalysis researcher.

However, in my sixth year on the faculty, my research went in a new direction that directly stemmed from two unexpected events, things that were never part of my plan. The first was my growing interest in separations, an area of chemical engineering that I never thought much about as a PhD student or postdoc. Georgia Tech has an exceptionally strong group of faculty studying separations, and as a member of the intellectual community, I was often on PhD thesis committees and heard lectures or seminars from students in other groups in my department. With significant exposure to the membrane groups of Bill Koros and Sankar Nair, as well as the combined solvents group of Chuck Eckert and Charlie Liotta, I began to think about how my group's materials might be employed in separation applications. Furthermore, at the time, our school did not have anyone studying adsorptive separations. To this end, in 2006, it seemed like starting projects in adsorptive separations might be a fruitful new direction for my group.

This new research theme was facilitated by an initial collaboration with Koros and Nair on membrane separations³⁴ and an inquiry from researchers at the DOE National Energy Technology Laboratory (NETL) about using the supported amine materials (Figure 1) we had developed as supports for polymerization catalysis^{35,36} in adsorptive CO₂ separations. That year, 2006, was the launching point for a research direction that now represents half my research program, a direction that I never would have imagined as a PhD student, postdoc, or even new assistant professor, one that stemmed from seizing unexpected opportunities that were presented.

Development of Research Themes

After promotion and tenure in the US academic system, but before promotion to full professor, is a good time to focus on development of core research themes. As noted above, in this period I began exploring the design of materials for separations as a research theme that was linked to my primary theme of catalysis and reaction engineering through the common component of synthetic materials chemistry. However, this was a new field for my group, a field in which we were unknown to the scientific community and had no credibility. Our approach to making inroads into the new field was to analyze the state-of-the-art at the time,² and also assess how we could make unique and meaningful contributions using our specific materials chemistry skills.

CO_2 separation as a theme

Of the variety of gas separation problems in which other researchers in my school were engaged, one that intrigued me right away was CO_2 separation from flue gases associated with fossil fuel combustion. This was not a topic widely studied by my peers at Georgia Tech at the time, and a literature review suggested that there were relatively few chemical engineers in academia in the United States engaged in this topic.² Furthermore, globally, those researchers who were engaged in the topic appeared to be chemical engineers who studied

commercially available materials, doing excellent engineering work on materials that I personally found boring, or materials scientists making interesting new materials whose gas separation properties were not being characterized in a way that most chemical engineers would call rigorous. To this end, it appeared that our group could make a real contribution to developing new materials for adsorptive separations by leveraging our budding knowledge of separations, drawn from numerous collaborations within Georgia Tech, and our materials design and synthesis skills. We chose to focus on supported amine materials (Figure 1) for CO_2 separation from flue gas as an initial theme.

Our first publication on supported amine materials for CO_2 capture from simulated flue gas leveraged our expertise discussed above in polymerization and silica chemistry, creating a new adsorbent through *in situ* polymerization of aziridine within the pores of a mesoporous silica while simultaneously grafting it onto the surface of the support.^{37,38} This material had improved CO_2 capacity and stability to humidity relative to other materials known at the time and provided a foundation for further research with our collaborator at NETL, McMahan Gray. To further establish the group in this new area, we undertook the writing of a comprehensive review on adsorbent materials for CO_2 capture from flue gas,² an approach we used previously¹ to both understand the global state of a new topic for the group as well as to establish ourselves as active researchers within the field.

As noted above, one reason we were able to get a fast start in separations was due to the number of other researchers studying separations in my school. By 2011, there was a broad array of other groups working in gas separations in my department, including the groups of Eckert/Liotta, Yoshiaki Kawajiri, Koros, Nair, Matthew Realff, David Sholl and Krista Walton. This enabled us to build a comprehensive team to study the implementation of supported amine adsorbents in a new type of scalable gas/solid contactor for separation of CO₂ from flue gas. Building on the development of rapid temperature swing adsorption (RTSA) by Koros and Ryan Lively (when he was a PhD student),³⁹ we developed methods to deploy supported amine adsorbents in hollow fiber contactors⁴⁰⁻⁴² that acted as microscopic shell-and-tube heat exchangers. Kawajiri and Realff explored and optimized the overall process while modeling the heat and mass transfer on the single fiber and separation module level.^{43–45} These fibers are in fact ideally suited for strongly chemisorbing sorbents such as supported amines, as they provide a unique opportunity for recovery of the heat of adsorption for possible integration into the rest of the capture process.⁴⁶ By the end of this project in 2014, we were able to make an impact on the field by combining sophisticated materials chemistry with process engineering expertise, in line with our initial goals.

CO₂ capture from ambient air

In 2008, my group was asked if we could design adsorbents that could efficiently extract CO_2 out of the ambient air. This type of separation challenge, concentrating a gas that is ultradilute (400 ppm) and present on a large scale, is one that many researchers well-versed in gas separations might have disregarded. Unhindered by long experience in separations, we said yes, thinking that the supported amine materials that the group had developed would be able to effectively do this. These materials, with their high heats of adsorption, provide a strong driving force for CO_2 capture, manifesting in a steep adsorption isotherm even at low CO_2 partial pressures.^{5,47}

Carbon capture has been discussed for decades as an approach to minimize emissions from fossil fuel combustion to mitigate some of the risks associated with climate change. In the most conventional sense, carbon capture strategies focus on large point sources associated with energy generation (coal or gas fired power plants) or other large industrial sources.^{2,48,49} However, if the emissions from such sources were captured and sequestered, this approach would still only address about one to two thirds of total emissions. Many sources, such as the hundreds of millions of small or mobile sources (planes, ships, trucks, etc.) are comparatively harder to address. In this regard, the ability to directly extract CO₂ from the air-direct air capture (DAC)-is a potentially paradigm changing technology. $^{6,50-52}$ Such a technology could be stationed anywhere in the world, for example, near sequestration or CO2 use sites, and could in principle address all global emissions. However, to date, without a global price on carbon and international agreement on emissions reductions, it is challenging to assess if such a technology could be feasible on a large scale. To this end, my group is working in collaboration with a start-up company, Global Thermostat LLC, to develop and test sorbents and processes that can allow for DAC on a large scale with substantially reduced costs.

Above, I remarked on the importance of working on *the* problem in a field, rather than simply *a* problem. While this is easy to state as a principle, it is quite hard to do in practice, and over the course of my career as a researcher we have worked almost exclusively on problems that advance the field in more modest ways. Our work targeting materials and processes for DAC is one of the rare paradigm-shifting problems in which our group is heavily engaged. In this regard, it is a topic of high risk, one where many contemporaries thought research was not needed.⁵³ However, such problems are well suited for inclusion in an academic researcher's portfolio of projects, because if universities do not work on such problems, who will?

Molecular and materials design and linkage between catalysis and separations

After a dozen years at Georgia Tech, my research program was well-developed and operating at steady-state. Synthetic materials chemistry provided the topical bridge between the two major research themes of catalysis and adsorptive separations. This somewhat nontraditional combination of two research foci—catalysis and separations research, which is historically carried out in separate communities within chemical engineering in the United States—has turned out to be highly synergistic.

As a research lab with an initial focus area of heterogeneous catalysis, the transition into adsorptive separations was quite straightforward. The group was already accustomed to thinking about the elementary steps in heterogeneous catalysis: (1) bulk, film and internal diffusion in solid materials, (2) adsorption, surface reaction and desorption from the surface, and (3) the reverse of the first steps, in our thinking about catalytic problems. On removal of the surface reaction step, these are

exactly the same key elementary processes in an adsorptive separation process. The group's expertise in materials design for catalytic purposes was easily transferable to adsorptive gas separations, and the laboratory was equipped for all the measurements needed to begin work in this field.

Furthermore, using silica-supported amines as platform materials in both research areas, the group was able to develop a deep, core expertise in a specific class of highly functional solids. The silica-supported amine fragment (Figure 1) was a key material that the first two students in my group used as a component of the ligand for their supported metal complexes in polymerization catalysis.^{35,54} These same materials have been used as basic organocatalysts, including in an ongoing study of acid-base, silanol-amine cooperativity in prototypical carbon-carbon bond forming reactions such as aldol and nitroaldol reactions.^{55–57} These materials and studies have directly intersected with parallel work using similar materials for CO_2 capture from dilute gases.^{58,59} The cooperativity of amines and silanols also appears to provide a pathway for CO₂ adsorption,^{56,60} though being of secondary importance to amineamine cooperativity to form more important alkylammonium carbamate structures that dominate CO₂ sorption from dry gas mixtures.4

Cross-fertilization of research ideas

In the highly collaborative environment in chemical and biomolecular engineering at Georgia Tech, there is substantial open cooperation and collaboration across different research groups. Additionally, in my research program, owing to the linking theme of synthetic materials chemistry and the presence of some common material platforms (e.g., silicasupported amines, Figure 1), researchers working primarily on separations also collaborate with researchers in catalysis and vice versa. Such open interactions lead to opportunities for new research directions. Two examples are given below.

Polymeric hollow fibers have been utilized for decades in membrane separations.⁶¹ Koros and Lively engineered these materials for adsorptive separations by creating mixed-matrix hollow fiber contactors,⁴⁶ which were later exploited in our postcombustion CO₂ capture project discussed above. As versatile fluid/solid contactors with the added ability to incorporate nanoparticle fillers, we envisioned that these hybrid materials could be used as microfluidic reactors in organic synthesis. To this end, as part of the Center for C-H Functionalization at Emory University, we demonstrated how silicaloaded polymeric fibers could be functionalized with molecular active sites for use as flow reactors in organic synthesis. Both enantioselective organometallic catalysts as well as simple organocatalysts, leveraging the group's catalysis expertise discussed above, were effectively deployed in flow using these polymeric fibers.62

The second direction involved the use of aminefunctionalized silica materials as adsorbents for volatile organic compound (VOC) removal from indoor air. Recognizing that the array of silica-supported amine materials that we had developed might also spontaneously adsorb and react with critical indoor air pollutants like formaldehyde, we partnered with the Dow Chemical Company to explore whether such materials could be made to efficiently trap this toxic vapor when it is present in indoor air in low concentrations. Our experience with such hybrid amine/oxide materials allowed us to create materials that efficiently trapped formaldehyde from dilute mixtures in air.^{63–65}

Both of the above examples demonstrate how a group with expertise in synthetic materials chemistry can leverage a few materials platforms for applied studies in several different topical areas in both catalysis and separations. The ability to work across multiple application areas provides the group with the ability to constantly introduce new research directions, and leverage funding sources targeting a variety of application areas. Furthermore, the students and postdoctoral researchers who are trained in the group enter the marketplace well equipped to work on a variety of problems applying materials chemistry expertise to problems in separations or catalysis and reaction engineering, distinguishing them from others who have more narrow experiences. Returning to the theme introduced above-building a research brand-an aspect of my laboratory's brand at this stage of my career is that we apply synthetic materials chemistry to address problems in both catalysis and adsorptive separations, a combination that while not unprecedented, is a bit unusual.

Summary and Advice for Researchers Beginning Their Independent Career

Building on the description of the evolution of my research program above, I close with a reiteration of some key advice for aspiring independent researchers.

1. Go in with a plan, but be ready to deviate; embrace new ideas and opportunities; a master plan may be impossible. A thoughtful plan is needed to land a job, but life is full of unexpected opportunities and challenges. You need to react to the challenges and seize the opportunities as they present themselves.

2. Know what makes you special as a researcher and person; use this as your lab's core, its center; there are some things you do better than most or all others. From this core, you can build and expand as new opportunities present themselves. In the example illustrated in this paper, the core was synthetic materials chemistry targeting well-defined molecular sites on surfaces, which was leveraged for myriad applications in catalysis and adsorptive separations.

3. Think outside your comfort area, embrace new directions, especially those that leverage your core. This is how a research program develops size and breadth. There is a critical minimum size that is important for the creation of good, internal scientific discourse. In times of tight research funding, the ability to expand application areas is critical to the creation of a solid research nucleus.

4. *Reflect often, be introspective*. Not only at the outset, but throughout your career, reflect often. Do not let imposter-syndrome cloud your judgement. All well-adjusted people will have moments of self-doubt. After 16+ years on the job I still leave conferences both inspired by the work of others, and also wishing I could do as beautiful (or deep, or inspiring, etc.) work as other researchers.

5. Create a positive, ambitious culture in your group; hire good people and get out of their way. Once a critical nucleus of researchers is built and the lab takes on a specific direction, the lab director largely gets to learn from the group, and the operation can become self-sustaining if productivity can be maintained.

The narrative description of the development of my research program provides an example and context for the major laboratory development stages described above: (1) the search for a position, (2) launching your laboratory, and (3) development of research themes. From my experience going through these three stages over the last decade and a half, the five elements of advice for emerging researchers above hopefully will prove useful to others embarking on an independent research career. In addition to these five elements of advice, I have complied a nonexhaustive list of other resources that may be helpful for an early career researcher, which is given in the Appendix A below.

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Literature Cited

- 1. Phan NTS, Van Der Sluys M, Jones CW. On the nature of the active species in palladium catalyzed Mizoroki–Heck and Suzuki–Miyaura Couplings homogeneous or heterogeneous catalysis, a critical review. *Adv Synth Catal*. 2006;348(6):609–679.
- Choi S, Drese JH, Jones CW. Adsorbent materials for carbon dioxide capture from large anthropogenic point sources. *ChemSusChem.* 2009;2(9):796–854.
- 3. Jones CW. CO₂ capture from dilute gases as a component of modern global carbon management. *Annu Rev Chem Biomol Eng.* 2011;2:31–52.
- Bollini P, Didas SA, Jones CW. Amine-oxide hybrid materials for acid gas separations. *J Mater Chem.* 2011; 21:15100–15120.
- Didas SA, Choi S, Chaikittisilp W, Jones CW. Amineoxide hybrid materials for CO₂ capture from ambient air. *Acc Chem Res.* 2015;48:2680–2687.
- 6. Sanz-Perez ES, Murdock CR, Didas SA, Jones CW. Direct capture of CO_2 from ambient air. *Chem Rev.* 2016;116(19):11840–11876.
- Delgass WN, Dumesic JA, Iglesia E, Ribeiro FH. Technical dedication: Michel Boudart special issue. J Phys Chem B. 2005;109:2035–2036.
- 8. Boudart M. Brief biographical sketch of Michel Boudart. *J Phys Chem B*. 2005;109:2037.
- 9. Bhan A, Iglesia E. A link between reactivity and local structure in acid catalysis on zeolites. *Acc Chem Res.* 2008;41(4):559–567.

- Gounder R, Iglesia E. The roles of entropy and enthalpy in stabilizing ion-pairs at transition states in zeolite acid catalysis. *Acc Chem Res.* 2012;45(2):229–238.
- 11. Bligaard T, Nørskov JK, Dahl S, Matthiesen J, Christensen CH, Sehested J. The Brønsted–Evans– Polanyi relation and the volcano curve in heterogeneous catalysis. *J Catal*. 2004;224(1):206–217.
- Abild-Pedersen F, Greeley J, Studt F, Rossmeisl J, Munter TR, Moses PG, Skúlason E, Bligaard T, Nørskov JK. Scaling Properties of Adsorption Energies for Hydrogen-Containing Molecules on Transition-Metal Surfaces. *Phys Rev Lett.* 2007;99(1):16105.
- 13. Hammer B, Norskov JK. Why gold is the noblest of all the metals. *Nature*. 1995;376(6537):238–240.
- Medford AJ, Vojvodic A, Hummelshøj JS, et al. From the Sabatier principle to a predictive theory of transitionmetal heterogeneous catalysis. *J Catal.* 2015;328:36–42.
- 15. Gladwell M. *Outliers: The Story of Success*, 1st ed. New York: Little, Brown and Company, 2008.
- Jones CW, Tsuji K, Davis ME. Organic-functionalized molecular sieves as shape-selective catalysts. *Nature*. 1998;393:52–54.
- Jones CW, Zones SI, Davis ME. m-Xylene reactions over zeolites with unidimensional pore systems. *Appl Catal A Gen.* 1999;181(2):289–303.
- Jones CW, Hwang S-J, Okubo T, Davis ME. Synthesis of hydrophobic molecular sieves by hydrothermal treatment with acetic acid. *Chem Mater.* 2001;13:1041–1050.
- Jones CW, Tsuji K, Takewaki T, Beck LW, Davis ME. Tailoring molecular sieve properties during SDA removal via solvent extraction. *Microporous Mesoporous Mater.* 2001;48(1):57–64.
- Jones CW. On the stability and recyclability of supported metal-ligand complex catalysts: myths, misconceptions and critical research needs. *Top Catal*. 2010;53(13):942–952.
- McKittrick MW, Jones CW. Toward single-site, immobilized molecular catalysts: site-isolated Ti ethylene polymerization catalysts supported on porous silica. *J Am Chem Soc.* 2004;126:3052–3053.
- Yu K, McKittrick MW, Jones CW. Role of amine structure and site isolation on the performance of aminosilicaimmobilized zirconium CGC-inspired ethylene polymerization catalysts. *Organometallics*. 2004;23:4089–4096.
- Nguyen JV, Jones CW. Design, behavior, and recycling of silica-supported CuBr-Bipyridine ATRP catalysts. *Macromolecules*. 2004;37:1190–1203.
- Nguyen JV, Jones CW. Effect of the synthetic method and support porosity on the structure and performance of silica-supported CuBr/pyridylmethanimine atom transfer radical polymerization catalysts. I. Catalyst Preparation and Characterization. *J Polym Sci Polym Chem.* 2004; 42(6):1367–1383.
- Schork FJ, Luo Y, Smulders W, Russum JP, Butté A, Fontenot K. Miniemulsion Polymerization. In: Masayoshi Okubo, editor. *Advances in Polymer Science*. Springer Berlin Heidelberg, 2005:129–255.
- Russum JP, Jones CW, Schork FJ. Continuous reversible addition-fragmentation chain transfer polymerization in miniemulsion utilizing a multi-tube reaction system. *Macromol Rapid Commun.* 2004;25(11):1064–1068.

- Qi G, Jones CW, Schork FJ. RAFT inverse miniemulsion polymerization of acrylamide. *Macromol Rapid Commun*. 2007;28(9):1010–1016.
- Smulders WW, Jones CW, Schork FJ. Synthesis of block copolymers using RAFT miniemulsion polymerization in a train of CSTRs. *Macromolecules*. 2004;37:9345–9354.
- South CR, Burd C, Weck M. Modular and dynamic functionalization of polymeric scaffolds. *Acc Chem Res.* 2007;40:63–74.
- Weck M, Jones CW. Mizoroki-Heck coupling using immobilized molecular precatalysts: leaching active species from Pd Pincers, Entrapped Pd Salts, and Pd NHC complexes. *Inorg Chem.* 2007;46:1865–1875.
- Yu K, Sommer W, Richardson JM, Weck M, Jones CW. Evidence that SCS Pincer Pd(II) complexes are only precatalysts in Heck catalysis and the implications for catalyst recovery and reuse. *Adv Synth Catal*. 2005;347(1):161–171.
- Madhavan N, Jones CW, Weck M. Rational approach to polymer-supported catalysts: synergy between catalytic reaction mechanism and polymer design. *Acc Chem Res.* 2008;41(9):1153–1165.
- Zheng X, Jones CW, Weck M. Ring-expanding olefin metathesis: a route to highly active unsymmetrical macrocyclic oligomeric co-Salen catalysts for the hydrolytic kinetic resolution of epoxides. J Am Chem Soc. 2007; 129:1105–1112.
- Bae T-H, Liu J, Lee JS, Koros WJ, Jones CW, Nair S. Facile high-yield solvothermal deposition of inorganic nanostructures on zeolite crystals for mixed matrix membrane fabrication. *J Am Chem Soc.* 2009;131:14662–14663.
- McKittrick MW, Jones CW. Toward single-site functional materials - Preparation of amine-functionalized surfaces exhibiting site-isolated behavior. *Chem Mater*. 2003;15:1132–1139.
- McKittrick MW, Jones CW. Modulating the reactivity of an organometallic catalyst via immobilization on a spatially patterned silica surface. *Chem Mater.* 2005;17: 4758–4761.
- 37. Hicks JC, Drese JH, Fauth DJ, Gray ML, Qi G, Jones CW. Designing adsorbents for CO₂ capture from flue gas-hyperbranched aminosilicas capable of capturing CO₂ reversibly. *J Am Chem Soc.* 2008;130:2902–2903.
- Jones CW, Hicks JC, Fauth DJ, Gray ML. Structures for capturing CO₂, methods of making the structures, and methods of capturing CO₂. 2012, US Patent 8,298,986.
- Lively RP, Chance RR, Kelley BT, et al. Hollow fiber adsorbents for CO₂ removal from flue gas. *Ind Eng Chem Res.* 2009;48:7314–7324.
- Rezaei F, Lively RP, Labreche Y, et al. Aminosilanegrafted polymer/silica hollow fiber adsorbents for CO₂ capture from flue gas. ACS Appl Mater Interfaces. 2013; 5(9):3921–3931.
- Labreche Y, Lively RP, Rezaei F, Chen G, Jones CW, Koros WJ. Post-spinning infusion of poly(ethyleneimine) into polymer/silica hollow fiber sorbents for carbon dioxide capture. *Chem Eng J.* 2013;221:166–175.
- 42. Fan Y, Labreche Y, Lively RP, Koros WJ, Jones CW. Dynamic CO₂ adsorption performance of internally cooled silica supported poly(ethylenimine) hollow fiber sorbents. *AIChE J*. 2014;60:3878–3887.

- 43. Kalyanaraman J, Fan Y, Lively RP, et al. Modeling and experimental validation of carbon dioxide sorption on hollow fibers loaded with silica-supported poly(ethylenimine). *Chem Eng J.* 2015;259:737–751.
- 44. Fan Y, Kalyanaraman J, Labreche Y, et al. CO₂ Sorption performance of composite polymer/aminosilica hollow fiber sorbents: an experimental and modeling study. *Ind Eng Chem Res.* 2015;54:1783–1795.
- 45. Rezaei F, Swernath S, Kalyanaraman J, Lively RP, Kawajiri Y, Realff MJ. Modeling of rapid temperature swing adsorption using hollow fiber sorbents. *Chem Eng Sci.* 2014;113:62–76.
- 46. Lively RP. Hollow fiber sorbents for post-combustion CO₂ capture. PhD Thesis, Georgia Institue of Technology, 2011.
- 47. Choi S, Drese JH, Eisenberger PM, Jones CW. Application of amine-tethered solid sorbents for direct CO₂ capture from the ambient air. *Environ Sci Technol*. 2011;45:2420–2427.
- 48. Aaron D, Tsouris C. Separation of CO₂ from flue gas: a review. *Sep Sci Technol.* 2005;40(1):321–348.
- 49. Balat H, Oz C. Technical and economic aspects of carbon capture and storage a review. *Energy, Explor Exploit.* 2007;25(5):357–392.
- 50. Zeman FS, Lackner KS. World Resource Review. 2004; 16(2):157–172.
- Pielke RA. An idealized assessment of the economics of air capture of carbon dioxide in mitigation policy. *Envi*ron Sci Policy. 2009;12(3):216–225.
- 52. Keith DW, Ha-Duong M, Stolaroff JK. Climate strategy with CO₂ capture from the air. *Clim Change*. 2006;74(1–3):17–45.
- 53. Society AP. Direct Air Capture of CO₂ with Chemicals: A Technology Assessment for the APS Panel on Public Affairs, 2011.
- Nguyen JV, Jones CW. Effect of the synthetic method and support porosity on the structure and performance of silica-supported CuBr/pyridylmethanimine atom transfer radical polymerization catalysts. II. Polymerization of methyl methacrylate. *J Polym Sci Polym Chem.* 2004; 42(6):1384–1399.
- 55. Brunelli NA, Venkatasubbaiah K, Jones CW. Cooperative catalysis with acid–base bifunctional mesoporous silica: impact of grafting and co-condensation synthesis methods on material structure and catalytic properties. *Chem Mater.* 2012;24:2433–2442.
- 56. Brunelli NA, Didas SA, Venkatasubbaiah K, Jones CW. Tuning cooperativity by controlling the linker length of silica-supported amines in catalysis and CO₂ capture. *J Am Chem Soc.* 2012;134:13950–13953.
- 57. Collier VE, Ellebracht NC, Lindy GI, Moschetta EG, Jones CW. Kinetic and mechanistic examination of acidbase bifunctional aminosilica catalysts in aldol and nitroaldol condensations. *ACS Catal.* 2016;6(1):460–468.
- Bollini P, Brunelli NA, Didas SA, Jones CW. Dynamics of CO₂ adsorption on amine adsorbents. 2. Insights into adsorbent design. *Ind Eng Chem Res.* 2012;51(46):15153–15162.
- 59. Alkhabbaz MA, Bollini P, Foo GS, Sievers C, Jones CW. Important roles of enthalpic and entropic contributions to CO_2 capture from simulated flue gas and ambient air using mesoporous silica grafted amines. *J Am Chem Soc.* 2014;136(38):13170–13173.

- Yoo C-J, Lee L-C, Jones CW. Probing intramolecular versus intermolecular CO₂ adsorption on amine-grafted SBA-15. *Langmuir*. 2015;31(49):13350–13360.
- Gabelman A, Hwang S-T. Hollow fiber membrane contactors. J Membr Sci. 1999;159(1–2):61–106.
- 62. Moschetta EG, Negretti S, Chepiga KM, Brunelli NA, Labreche Y, Feng Y, Rezaei F, Lively RP, Koros WJ, Davies HML, Jones CW. Composite polymer/oxide hollow fiber contactors: versatile and scalable flow reactors for heterogeneous catalytic reactions in organic synthesis. *Angew Chem Int Ed.* 2015;54(22):6470–6474. doi:10.1002/ anie.201500841.
- 63. Nomura A, Jones CW. Airborne aldehyde abatement by latex coatings containing amine-functionalized porous silicas. *Ind Eng Chem Res.* 2015;54(1):263– 271.
- 64. Nomura A, Jones CW. Enhanced formaldehyde-vapor adsorption capacity of polymeric amine-incorporated aminosilicas. *Chem Eur J*. 2014;20(21):6381–6390.
- 65. Nomura A, Jones CW. Amine-functionalized porous silicas as adsorbents for aldehyde abatement. ACS Appl Mater Interfaces. 2013;5(12):5569–5577.

Appendix A: Early Research Career Resources from Other Authors

• Barker, K.; At the Helm, A Laboratory Navigator, Cold Spring Harbor Laboratory Press: New York, 2002. Barker, K.;

At the Helm, Leading Your Laboratory, Cold Spring Harbor Laboratory Press: New York, 2010. ISBN 978–0879698669. This resource is rich with useful information. In addition to holding a group copy of this book, I recommend that all my students and postdocs interested in leading a research laboratory buy a copy of this book.

• C&E News recently published a useful piece describing the experiences of 3 new chemistry faculty: http://cen.acs. org/year-in-the-life-of-a-new-professor.html#body Other, related articles have appeared in the past: http://cen.acs.org/ articles/92/i36/New-Chemistry-Professors-Share-Experiences. html These articles provide useful resources as well.

• In 2015, Elsevier connect published a piece on *Tips for success on your path to tenure*, by Rodney E. Rohde: https://www.elsevier.com/connect/tips-for-success-on-your-path-to-tenure

• Kelsky, K.; *The Professor Is In: The Essential Guide To Turning Your Ph.D. Into a Job*, Three Rivers Press: New York, 2015. ISBN 978–0553419429

• Johnson, A. M.; *Charting a Course for a Successful Research Career*, Elsevier: Amsterdam, 2011. ISBN 978–90-817200–1-4 https://www.elsevier.com/_data/assets/pdf_file/0013/90040/charting-a-course-for-a-successful-research-career.pdf

A simple internet search will uncover an array of additional resources as well. While some advice is generic to any research position, other resources are specialized. The reader should realize that many pieces focus on specialized positions, and not all advice is universal.