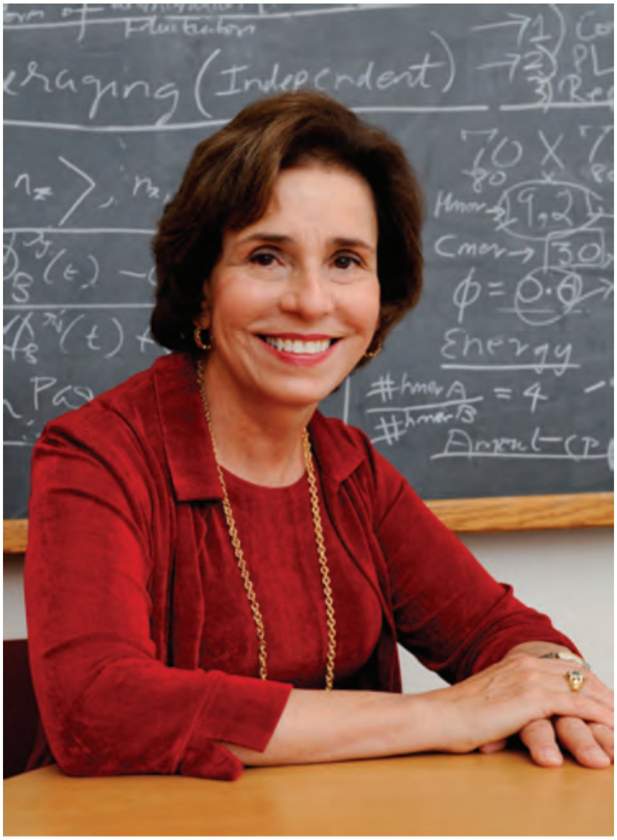

Carol K. Hall

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A ChemE Grows in Brooklyn

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Abstract

I profile my personal and professional journey from being a girl of the 1950s, with expectations typical for the times, to a chemical engineering professor and still-enthusiastic researcher. I describe my family, my early education, my college and graduate school training in physics, my postdoc years in chemistry, and my subsequent transformation into a chemical engineering faculty member—one of the first women to be appointed to a chemical engineering faculty in the United States. I focus on the events that shaped me, the people who noticed and supported me, and the environment for women scientists and engineers in what some would call the "early days." My initial research activities centered on applications of statistical mechanics to predict phase equilibria in simple systems. Over time, my interests evolved to focus on applying molecule-level computer simulations to systems of interest to chemical engineers, e.g., hydrocarbons and polymers. Eventually, spurred on by my personal interest in amyloid diseases and my wish to make a contribution to human health, I turned to more biologically oriented problems having to do with protein aggregation and protein design. I give a candid assessment of my strengths and weaknesses, successes and failures. Finally, I share the most valuable lessons that I have learned over a lifetime of professional and personal experience.

INTRODUCTION

Some people, like my partner, Sheldon, or my friend Francis Arnold, charge through life. They are brave, know where they want to go, and do what they need to do to get there. Not me!

I was brought up to be good, sweet, and pretty—to get married, and to have children. Those were the expectations for girls growing up in Brooklyn, New York, in the 1950s. My teachers wrote in my PS 225 elementary school yearbook, "Ever so pretty, smile so bright, Carol makes sunshine, come out at night" (**Figure 1**). (I still feel good about that!) Drive, determination, and ambition were for boys. Competition made me uncomfortable; it never occurred to me to be ambitious. I excelled at meeting the expectations of my era. I went to college because everyone went to college. I majored in physics because my physics teacher told my mother, "Girls can be physicists too." I got married shortly after college graduation because that was what you were supposed to do. I went to graduate school because my husband was going and I wasn't ready to start a family.

Figure 1

Carol M. Klein; childhood portrait, age unknown.

Nevertheless, a few things happened over the subsequent half century, and I wound up having a wonderful career, acquiring drive and determination (slowly), and making a mark of sorts in the world. (Note the modesty—good little girls of the 1950s who bragged eventually had no friends.) I agreed to write this autobiography, even though it could be construed as bragging, because I thought it might reassure younger people, particularly women, that it is possible to have a successful career even if you don't start out as the most confident or driven person in the world, or have a clear career path in mind.

GROWING UP IN BROOKLYN, NEW YORK

My father, Harris J. Klein, was a big shot. Though 5'5", he was a larger-than-life character—the kind of person that people liked to be around (**Figure 2**). The fifth of six sons of a Jewish couple

Figure 2

Harris and Celia Klein.

who emigrated from Galicia (a region in the Austro-Hungarian Empire) to the United States around the turn of the twentieth century, he grew up on the Lower East Side of New York City. He was an amateur boxer; hawked canaries on the Bowery, assuring customers that the females could sing (they can't); and held his own in a world of tough guys. He went to Brooklyn Law School, started his own law firm and other businesses, and got involved in politics. A lifelong Democrat, he was the campaign manager for Estes Kefauver (Adlai Stevenson's vice-presidential running mate in 1956) and for New York City mayors Robert Wagner and Abe Beame. I remember accompanying my dad on a nighttime trip to Gracie Mansion when I was 12. I conversed politely with Mayor Wagner's son while our fathers shouted at each other in the next room. My father was the dinner chairman for President Kennedy's birthday dinner at Madison Square Garden in New York City, where Marilyn Monroe, in a skintight dress, sang, "Happy Birthday, Mr. President." I was in the audience, and even I (a naive 16-year-old) sensed that something was going on between them. I also liked the dress! Daddy was a NYC Transit Commissioner, one of five men who ran the subways, and he ran (unsuccessfully) for Brooklyn borough president in 1957 in the Democratic Primary. His campaign promise was to keep the fare at a nickel.

My mother, Celia Reitman Klein, was the daughter of an immigrant Jewish couple, also from Galicia, who arrived in New York City at the turn of the century. Her father, Abraham, had deserted from the Czar's army, fleeing to the United States because Jews did not last long in the military. "Papa" was a highly skilled tailor who worked for a time in the Saks Fifth Avenue ladies department. The Depression was brutal for him, my grandmother, Dora ("Mama"), and their nine children, punctuated by brief periods of hunger and of homelessness. My mother, Celia, and her siblings all went to work once they were old enough to hold a job. A tall girl, my mother was proud of her ability to run fast, her academic abilities, and her street smarts. She graduated from high school with a secretarial degree and went to work in my father's law office when she was 16 and he was 28. She married him 11 years later, after he divorced his first wife (the mother of my two half-sisters). My mother was very smart and read constantly but, being a good wife of the 1950s, did not work outside of the home while my younger brother Mitchell and I were growing up. She went back to school in her sixties, earned a liberal arts degree from Brooklyn College, and then went to work for the probation department in the NYC prison system.

I went to the local public elementary and high schools in Brooklyn. My parents wanted me to attend private school, but I resisted because it was an all-girls school and I liked boys (**Figure 3**). When left on my own, I played "school," teaching my dolls how to read even before I knew how to do it. Every Sunday we drove to Mama and Papa's house, where my younger brother, Mitchell, and I played with our many cousins and kibitzed (kidded around) with my aunts and uncles. In summer, I went to a Jewish girls' sleepaway camp, where I worked to earn stripes for table manners, sportsmanship, and character. My favorite grade was the fifth grade—my recollection is that we mainly sang, danced, and painted pictures. According to my mother, we also learned math. It was around then that I surpassed my parents' ability to do math—when I explained to them that to divide fractions you had to turn the denominator upside down and then multiply, they declared me wrong. In the afternoon, after school let out, I was educated in the arts. I took ballet and modern dance lessons twice a week (from Marjorie Mazia, a Martha Graham dancer who was married to famed folk singer Woody Guthrie), piano lessons every Sunday morning, and oil painting lessons every Wednesday night (the only child in the class). Five boys asked me to the elementary school prom—probably a record. (Maybe I was already channeling the 1950s girl's expectation to "get married," or maybe I just liked boys.) Neil Sedaka, a PS 225 alum, sang at our prom.

Sputnik, which was launched by the Russians when I was in seventh grade (in 1957), had a big impact on my education and on my life. The first man-made satellite, *Sputnik* caught everyone in the United States off guard. People were afraid of the Russians. The atmosphere was exacerbated

Figure 3

On road to meeting expectations (?) for girls of the 1950s.

by in-school air-raid drills where we were instructed to hide under our desks in case of a nuclear attack. *Sputnik* galvanized the teachers in the New York City public school system, who saw it as their mission to urge their brightest students to become scientists so that we could "beat the Ruskies." I had no interest in science at the time (I mainly liked singing, dancing, and painting), but by the ninth grade (my first year in high school), some of the science message must have sunk in. I had a recurring dream. I was in gym class, wearing the required ugly green gym suit, when it was announced on the school loudspeaker that all students would be sent to the gas chamber unless they pledged that they would go into science. In the dream, I immediately leaped up to grab the nearest wall phone and called my parents to tell them not to worry—I would go into science. The dream occurred several times each night and lasted for months. I have no idea how my subconscious amalgamated science with the Holocaust. Perhaps it was that I had made new friends in high school whose parents were Holocaust survivors. I was very aware that all of the members of my extended family who had not emigrated to the United States died in the concentration camps. I am not saying that I made a decision to *be* anything at the time—girls were not expected to have careers—but somewhere along the way this dream must have influenced my career choice.

My high school, Abraham Lincoln High School, was near Coney Island in Brooklyn and boasted more than 5,000 students. The teachers were dedicated to providing a superb education. Lincoln boasts three Nobel Prize winners (two in chemistry); two Pulitzer Prize winners; and a host of celebrities, including Mel Brooks, Neil Diamond, and Arthur Miller. Most of the children were Jewish, a minority were Italian, and a few were African American. In ninth, tenth, and eleventh grades, I did my best to blend into the background. The only time I stuck my neck out was to try out (unsuccessfully) for cheerleaders and for pom-pom girls—those were for the prettiest and most vivacious girls. I made new friends with smart girls who were serious about academics and did very well in all my classes, except French. I loved the math class—math came easily to me and I thought it was a beautifully logical subject—nearly as much fun as dancing and art. I took physics in my junior year from Dr. Herman Gewirtz and advanced physics with him the next year. One open school night, he told my mother that in college I should major in physics. When my mother expressed skepticism, he assured her, "Girls can be physicists too."

During my senior year, I had a bit of a personality change. I was tired of being a follower, so I ran for vice president of our senior class. (Girls were not allowed to run for president, a position reserved for boys.) My campaign promise was that the senior class would sponsor an underprivileged child living in China, named Chan Sing Lee, through the Foster Parents Plan. My opponent was a basketball player, Jeffrey, who was very tall and about as shy as I was. I am not sure why I won—maybe Jeffrey missed too many baskets. I enjoyed being senior class vice president and became more outgoing. I still sponsor children through the Foster Parents Plan.

COLLEGE

Cornell was a completely new world for me—intimidating at first and frankly, later on as well. Although there were a fair number of Jewish students there, they (we) were not in the majority; this was an atmosphere that I was not used to. Some of the students were from wealthy "high society" families, and I could tell that they were in a different league than me. My very first date (they were very big on dating there) was a boy I met in the campus bookstore who walked me back to my dorm room and asked me if Jews really had horns. My second date, a junior my dorm counselor fixed me up with, took me to a fraternity party and urged me to drink a large glass of whisky (I did), causing me to spend the evening in the bathroom being sick. At the convocation for my entering freshman class, the then-new Cornell University president, James Perkins, said, "Look to your left, look to your right—one of you won't be here for graduation." He was right.

Being the good girl that I was, I did as my mother advised and majored in physics. There were 40 physics majors at Cornell in my freshman class (6 girls and 34 boys) and 12 physics majors at graduation (6 girls and 6 boys). Having such a large number of female physics majors was completely unheard of then and is still far from the norm. The reason we girls stayed the course was that we supported each other and bonded. The math classes were my favorite classes—I did well in those. The physics classes were hard—I was a B to B+ student, which was respectable in those days. Timed tests made me anxious—I did not (and still do not) think fast and did not work well under pressure. However, when the tests were very hard and I sensed that the other students thought it was hopeless, I relaxed and did well. For the most part, my classmates and I were ignored—the physics faculty were mostly interested in their research. Nobel Prize winner Hans Bethe threatened to fail our entire modern physics class but was talked out of it by the department head. One bright spot was my freshman physics advisor, David Lee, who cooed to his young children on the phone during my advising appointments with him and reassured me senior year that all would be okay after I did badly on his statistical mechanics final. David Lee won the 1996 Nobel Prize in Physics. And I became a statistical "mechanician."

How much did I care about grades? They were somewhat important to me, but not a lot. I was much more interested in boys, which is where the competition was. We girls essentially competed with each other to have dates and to find boyfriends who were "cute." I dated in my first two and a half years; met my (now-former) husband, Tom Hall, in a physics class during junior year; became engaged at the end of my senior year; and married the August after graduation. As a matter of fact, most of the 14 girls who had been on my freshman dorm hall married their boyfriends that summer. Many of those marriages ended in divorce. Tom and I divorced 10 years ago after 40 years of marriage and three children.

GRADUATE SCHOOL

Tom and I went to graduate school in physics at the State University of New York at Stony Brook. Stony Brook was a fairly new university with an excellent physics department, boasting C.N. Yang, a Nobel Prize winner, on the faculty. I did better in my physics classes as a grad student than I did as an undergraduate. Maybe they were better taught and more math oriented—or maybe I was just growing up and allowing myself to be more interested. After all, I had already fulfilled the 1950s girl's expectation of getting married; there was nothing left to prove.

Physics majors took classes in their first and second year and were assigned to thesis advisors at the start of their third year. Professor X (who shall remain nameless) invited me to join his group. He was doing experiments on critical phenomena (the behavior in the vicinity of the critical point of a phase transition), and the subject interested me. I had heard a seminar on critical phenomena (1) by Michael Fisher (a Cornell professor and later one of my postdoc advisors) and loved that the peculiar behavior in the vicinity of the critical point applied to so many seemingly unrelated systems: liquids, ferromagnets, binary mixtures, etc. The other benefit of working in Professor X's group was that I could improve my experimental skills, which were weak.

I joined Professor X's group at the beginning of my third year at Stony Brook. We conducted experiments on critical phenomena, shining laser light through a transparent cell containing argon gas while its temperature was raised from below to above its critical point. By monitoring the change in the index of refraction, we could measure the critical exponent beta. Many a day was spent in our basement lab in a darkened room watching laser beams flash around as the more senior grad student took measurements. Eventually, Professor X asked me to write programs to automate the recording and analysis of optical data. That was fun. The music stopped, so to speak, about a year later. Tom and I were at a graduate student party at the home of Professor and Mrs. X. Music was playing, there was a fair amount of drinking (not by me) and dancing. Professor X asked me to dance, danced me into a nearby room, and kissed me full on the mouth, which was a big surprise. I realized immediately that this was a bad situation and that my days in Professor X's group needed to be over. I contacted the Director of Graduate Studies, Professor Max Dresden, one of my favorite professors, and he helped me to find another advisor. Today, as a result of the #MeToo movement (2), Professor X would be disciplined and likely fired, but in those days his failed attempts at flirtation/seduction were a source of amusement. The department was not a hostile environment for women, because most people were nice (although one of my mechanics homeworks did ask us to model the simple harmonic motion of a woman's breasts). They were just insensitive and oblivious like the rest of society at the time.

Professor Dresden suggested that I talk to a new professor, George Stell (3), who had just been hired by the Department of Mechanics at Stony Brook and whose subject area was statistical mechanics (**Figure 4**). Stell came from the Polytechnic Institute of Brooklyn, where he had been an associate professor, and had not had a graduate student before. A big, friendly man, with a scruffy beard, thick glasses, and a ready laugh, Stell was what we called a hippie in those days. I went to see him, described what had happened with Professor X (which he found amusing), and explained that I was looking for a new advisor. He described his research at great length, and much to my delight, it was about phase transitions, which seemed to be in the scientific neighborhood of critical phenomena. At the end of our conversation, I blurted out that he probably wouldn't want me as a graduate student because I "wasn't very smart." Instead of saying the usual, "Of course you're smart, you are a fourth-year student in physics," he asked me, "How do you know?" When

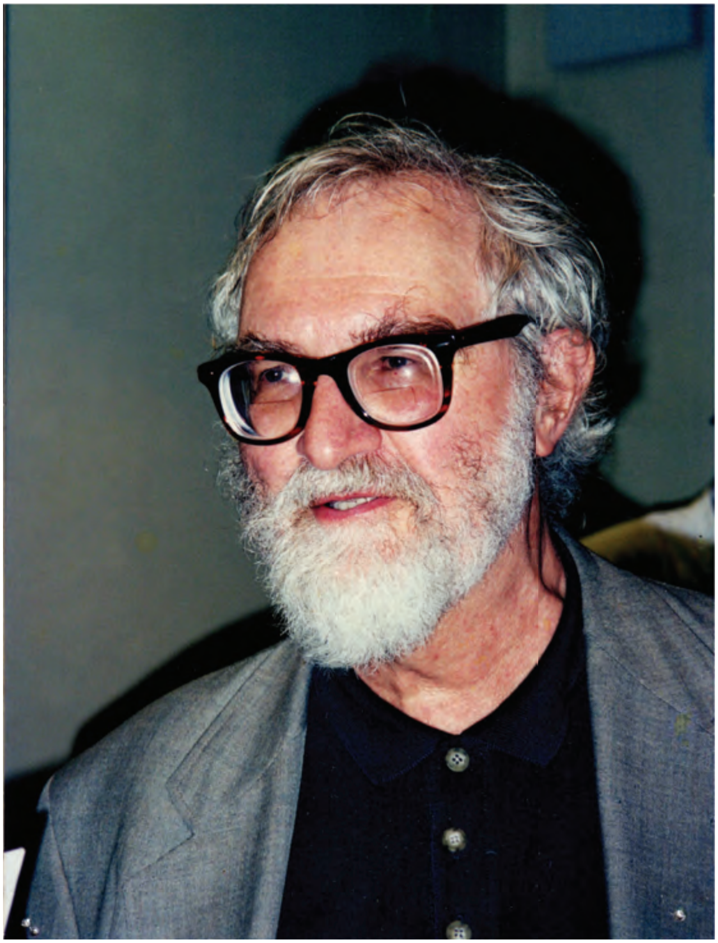

Figure 4

George Stell.

I responded, "I don't do that well on tests," he replied, "I don't give a f___ how you do on tests, can you do research?" I said, "I don't know," and he replied, "Well, let's find out." Stell agreed to take me on as a provisional student.

My first research meeting with Stell was memorable. We met at his house because, as he explained, he had a home office and all of his papers were there. I drove to his house and we met in a back room, complete with desk, bookshelves, and a bed. (His wife was not home at the time.) I was a little concerned, but he seemed fine and the research was interesting. At the end of our long meeting, in which he overwhelmed me with his research ideas, he jumped up and announced with a smile that he had something to show me. I was instructed to wait in the office, and he left the room. Given my previous experience, part of me expected him to come back minus his clothes. I was trying to figure out how to make my escape when he returned a few minutes later playing a big trombone and entertaining me with his jazz compositions.

Meeting Stell was probably the best thing that ever happened to me professionally. He didn't care that I was a girl or how well I did on tests; he just wanted to do research. Instead of competing with classmates to see who could solve a test problem first or fastest, I got to compete with the science. It was up to me to figure out how to tackle a problem that no one had ever solved before. I was even allowed to be creative! I fell in love with research. My PhD thesis, "Phase Transitions in Systems with Competing Interactions," examined how the relative strengths and ranges of repulsions and attractions in lattice gas models of fluids determine the types of phases (solid, liquid, and vapor) that will appear (4–6). George Stell became a lifelong friend. Sadly, he died in 2014. I was one of the trustees of his estate. I, and the many others with whom he worked, still miss him.

POSTDOC

After graduate school, it was time to find a job. A complicating factor was finding two postdoc positions in the same place—one for me and one for Tom, who had defended his PhD thesis the same day I did. I have a file of 40 rejection letters from that time. I applied for and received a National Research Council fellowship to work at the National Bureau of Standards, but Tom's fellowship application was not successful. He got a job offer at Brandeis University, but I did not. My dream was to postdoc with Ben Widom at Cornell, who was working in critical phenomena, but he was looking for an experimentalist who could measure tri-critical behavior. When Tom got a postdoc offer at Cornell's Materials Science Department, we decided that I would do a "voluntary postdoc" in the Widom group, which meant I would work full time but not get paid. Some people thought I was foolish—why work if you don't get paid?—but I considered it a golden opportunity to learn from the best. Our first child, Katie, was born the December after we arrived. I took a couple of months off after Katie's birth and then hired a full-time caregiver so that I could go to the office and learn to be a postdoc.

The Widom/Fisher lab was awe-inspiring. Widom's office was next door to that of Michael Fisher (a world-famous statistical mechanician), and they and their groups closely interacted. The grad students and postdocs were brilliant (not a word I often use) and deeply immersed in their subjects. The main topic of interest was critical phenomena: how to explain the nonclassical critical exponents that are found in nature. A frequent visitor to the group was Ken Wilson, a young professor in the Physics Department. I got to witness lively conversations between Widom, Fisher, and Wilson about a new idea, renormalization group theory, which won Wilson the 1982 Nobel Prize in Physics. My research with Ben culminated in two papers, one of which (7) was pretty esoteric: "Scaling in the Ideal Bose Gas" in greater than four dimensions. Note that that's four *spatial* dimensions!

BELL LABS

Our next positions were at Bell Laboratories; I worked in the Economics Modeling Department in Murray Hill, New Jersey, and Tom worked in the Device Development Department in Allentown, Pennsylvania. I stayed at Bell Laboratories for 13 months and 4 days. The work was interesting, but I couldn't figure out the politics there. My department head seemed to enjoy keeping me off balance and, when I left the labs, told me that I would "never amount to much." I did like my supervisor, Bernie, and learned about industrial engineering from him. Under his direction, I developed pricing strategies for Bell System products using a combination of Markov models and commonsense decision making. I found out later that my model was adopted by the Bell System.

PRINCETON

Two weeks after I joined Bell Laboratories, I got a call one evening from Barry Royce, a professor at nearby Princeton University. "Would I be interested in interviewing for an assistant professor

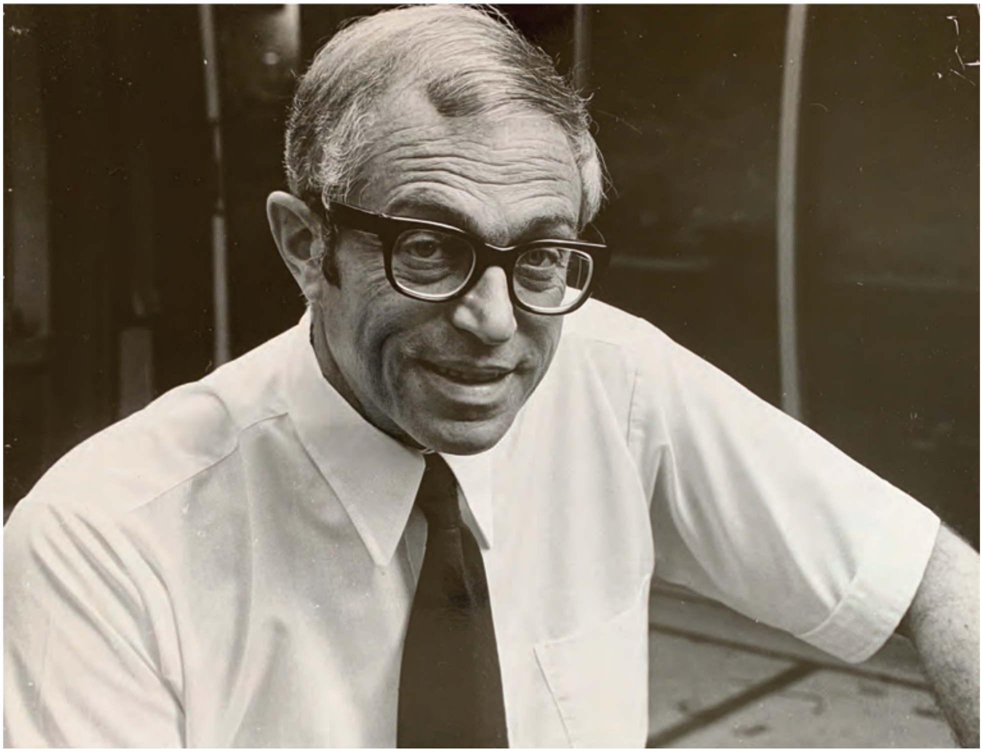

Figure 5

Leon Lapidus.

position in the Aeronautical and Mechanical Engineering Department at Princeton?" They had "heard that I was in the area." Here is where I showed uncharacteristic boldness and wisdom. Instead of saying, "I'm sorry, I just started working at Bell Labs and couldn't possibly think of moving after only two weeks," I told Royce I would be happy to visit. A month later, I gave a rousing seminar on my research in a large room to an audience of three people, one of whom left in the middle. I then met with the Head of the Aeronautical and Mechanical Engineering Department, and we discussed ways that I might fit in. (There weren't any!) Afterward, I informed my host, Dean of Engineering Robert Jahn, that I did not think it would work out. Jahn understood and asked only that I accept his periodic invitations to lunch at the Nassau Club, a gentleman's club reserved for "Old Tigers." Although women could not be club members, they could come to lunch. Because the food was good and Bob was fun to talk to, I accepted and joined him for lunch on several occasions over the next year.

Eventually, Dean Jahn introduced me to Leon Lapidus, the head of the Chemical Engineering Department (**Figure 5**). Leon was Jewish (we had that in common) and enthusiastic about hiring women faculty. His view was that if we can't grow our own, we ought to adopt them. In April, I again gave a seminar at Princeton, but this time to the Chemical Engineering Department. There was a sizable audience, and they asked good questions and seemed to like me. I met with most of the faculty and was offered a job as a tenure-track assistant professor, the first female professor in the Princeton College of Engineering and the third female chemical engineering faculty member in the nation. Leon told me not to worry about my lack of training in chemical engineering; chemical physics (which was what I studied) was close enough. He said he would teach me the jargon and

Figure 6

Princeton faculty and grads, April 1978, one month before Adam's birth.

help me to fit in. Sadly, on May 5, 1977, two months before my arrival, he suffered a massive heart attack in the office and died. He was only 52 years old.

I joined the Princeton Chemical Engineering Department on August 15, 1977. I was 31 years old. I remember walking alone into my office on my first day and finding it cold and barren, except for an ancient stapler on the desk and an ashtray in the shape of a rubber tire. There was a buzzer on the wall, and when I pressed it (*bumpety bump bump—bump bump*), someone in the building buzzed me back. This exchange continued during my entire stay at Princeton. I would play a little rhythm on the buzzer when I had the urge, and someone would answer back. I never figured out who. Welcome to Princeton!

What was it like being the first female professor in the ChemE Department at Princeton (**Figure 6**)? Challenging! I had been hired and championed by Leon (evidently a dominant figure), but he was no longer there, and I was on my own. I was different from the types of assistant professors that my colleagues were used to. (Suggested supplemental reading: Hans Christian Andersen's famous fairy tale, "The Ugly Duckling.") Although a few of the senior professors were quite welcoming to me, most were cool or ambivalent. I think they didn't know what to make of me—this strange female person who was trained in physics ("not one of us") and who, for goodness' sake, got pregnant just after she was hired. When rumors that I was pregnant started to circulate, the executive secretary, who ran the department, declared to all who would listen, "She [meaning me] wouldn't dare get pregnant." Surprise! (My son Adam was born in May of that year, and my daughter Norah was born in April of my fifth year at Princeton). One senior colleague, Professor Y, made disparaging remarks about my gender (e.g., "Everyone knows women can't do science") and my field ["The only applied mathematics worth doing is in XYZ (his field)"]. The grad students were reluctant to work with me; I didn't get my first one until my third year.

When I asked the new department head, Bill Schowalter, for his help and guidance, he demurred by saying he had to treat all of the assistant professors alike. I needed coaching (today we would call it mentoring) because I was different than the other assistant professors, but Schowalter seemed genuinely baffled by that concept. He finally suggested that I prove postulates in thermodynamics instead of working in statistical mechanics. I did receive advice from John Prausnitz, who visited during my first year. He expressed delight that Princeton ChemE now had a thermodynamicist (me) and suggested that I do research on polymers and supplement my theoretical work with experiments. When I told him that I was not good at experiments, he pointed out that it's the grad student, not the advisor, who does the experiments. When I asked him what I should do if the experiments didn't work, he said (with a twinkle in his eye), "Ask the student if it is plugged in." I eventually found a mentor: Keith Gubbins, a professor at Cornell University who is now my colleague at North Carolina State University (NC State) (**Figure 7**). I had called him because he had just written a textbook, *Applied Statistical Mechanics* (8), for ChemEs, and I was planning to teach a graduate course in statistical mechanics. Keith was very friendly, sent me his course notes, advised me to go to AIChE (American Institute of Chemical Engineers) meetings, and invited me to give a seminar at Cornell. Keith continues to mentor me, although I don't think he would call it that.

Teaching chemical engineering was an adventure. My first year, I was assigned to teach staged operations—I had no idea what that was. Fortunately, a kind colleague, Joe Calo, shared his course notes with me. Staged operations was so different from physics! The McCabe–Thiele diagrams tickled me because you needed to sharpen your pencil to get the most accurate answer. I was also assigned to teach the undergraduate laboratory and had responsibility for the double-effect evaporator, in which water was circulated through a huge (and ancient) system of pipes while being heated and cooled at different stages. One semester, I was even in charge of the whole lab. (Thank goodness for teaching assistants!) After a couple of years, I was asked to apprentice-teach the Thermodynamics I and II classes. Professor Richard Toner, a beloved Princeton professor who had taught that class for nearly 40 years, was about to retire. I became his head teaching assistant and taught problem sessions. The undergraduate students were incredulous, writing (for example), "How could a physicist possibly teach thermodynamics?" Once Toner retired and I took over Thermo I and II, I did well in my teaching evaluations. My favorite evaluation: "Like John Glenn, Professor Hall has the 'right stuff.'" I still love teaching thermodynamics to undergraduates.

I tried to "fit in." My strategy was sensible—be friendly, pleasant, and interested in others—but one of my efforts was, in hindsight, comical. On seminar days, Wednesdays, I would walk over to the Faculty Club with a bunch of other professors to eat lunch with the speaker. I noticed that nearly all of my colleagues were tall, lanky, and athletic (they played squash) and that they wore blue blazers and khaki pants. Well, I couldn't do much about my height, and squash was not in my skill set, but I could change the way I dressed. Maybe that would help me fit in? So, I went out and bought a lovely blue blazer and a khaki skirt and wore them on Wednesdays. And nobody but me noticed! It became easier to fit in when the department hired four new assistant professors: Robert Prud'homme, Jay Benziger, Sundar Sundaresan, and Jeff Koberstein. Although there was a little good-natured ribbing at first about who worked the most hours per week (all had stay-at-home wives who took care of their children), we all became friends rather quickly. I am still friends with them all.

Figure 7

Hall with Keith Gubbins and Geoff (a papier-mâché tiger).

Why am I so grateful that I had the opportunity to spend time at Princeton, and why am I dwelling on it in this autobiography? There are two reasons. First, it was a defining moment in my career—it shaped me. Princeton gave me an entrée into a new field, chemical engineering, that really suits me. It was, and still is, a gold mine of interesting problems that are crying out for the kinds of research techniques that I know how to do: molecular modeling, statistical mechanics, and computer simulation. Second, I got the freedom to explore my own research ideas and to do this with some great grad students, postdocs, and collaborators.

My first research project at Princeton was on modeling the behavior of hydrogen in metals. Metal hydrides, e.g., niobium hydride, are a physical realization of the types of lattice gas models that I investigated as a graduate student. They exhibit gas-like, liquid-like, and solid-like phases, depending on the amount of hydrogen that is absorbed. The phase transitions are a thermodynamic consequence of the effective attraction between the hydrogen atoms in the metal induced by the stretching/distortion of the host metal lattice. Metal hydrides were of interest because of the "hydrogen economy," the idea that hydrogen gas (which burns to produce water) could replace petroleum in cars and that it would be stored in a metal. Our approach was to use computer simulations, which were new to me, to predict these phase transitions. My first PhD student, Mauricio Futran, and I learned how to do Monte Carlo simulations together (9). He and the students that followed him at Princeton and later at NC State contributed to that field in a way that makes me proud (10–12). Mauricio is now a vice president at Janssen Pharmaceuticals and is a member of the National Academy of Engineering. He remains a good friend.

My second research project at Princeton was a joint effort with my colleague, then–associate professor Bill Russel, in the area of colloids. Bill was doing experiments on the flocculation (precipitation) of colloids by the addition of polymers and wanted to model this phenomenon. Asakura & Oosawa (13) had shown that adding polymers to a colloidal solution induced an effective attraction between the particles. I proposed that we model this effect using the statistical mechanics techniques that I had learned as a graduate student. Our student, Alice Gast (now president of Imperial College London), was quite sharp and quickly learned the theory and how to apply it. That work is considered significant (a citation classic) because it showed that statistical mechanics could be applied to systems that are not molecules and that it could predict the gas, liquid, and solid phases exhibited by colloid–polymer solutions (14). It also showed that the range of the colloid–colloid interaction, which can be changed by adding polymer, dictates whether or not the gas–liquid coexistence curve and accompanying critical point will be observed or be metastable. The latter point has been rediscovered by many investigators over the years, as it has relevance for the crystallization of globular proteins as well as colloidal suspensions (15, 16). Experiments in the Russel lab verified our predictions and our approach (17).

An interesting sidelight to my research at Princeton was my collaboration with Bell Laboratories scientist Eugene Helfand. Because my home was closer to Bell Labs than to Princeton, I sometimes spent time in their theoretical chemistry offices, where I met Gene, a theorist working in the polymers field. I asked him if he had any interesting mathematical problems to work on, and he put me to work. The result, after pages upon pages of equations, was an exact expression for the time correlation for polymer conformational relaxation. The Hall–Helfand correlation function has since become a standard against which to compare nuclear magnetic resonance relaxation and time-resolved fluorescence spectroscopy measurements. This is one of my most cited papers (18). Interestingly, I did not think it was a very good paper at the time.

On November 15, 1983, I learned that the senior faculty at Princeton had voted to deny me tenure. This was a blow and a surprise to many who knew me. When I came up for tenure, I had 27 papers in refereed journals, had raised nearly half a million in research dollars, and had a $100,000 grant pending and a total of seven students. Why do I think I was denied tenure? Two reasons. First, the not-one-of-us syndrome: I was a female and a physicist, and my research did not seem like chemical engineering to most of the faculty. Second, I was competing against my friend Bob Prud'homme, who was a strong scholar and the best fundraiser the department had ever seen. The scuttlebutt at the time was that if the department recommended both of us, the university would promote only one, and that would have had to be me because the university had been criticized for its treatment of women faculty. I spent my last year at Princeton searching for another academic job. Interestingly, some of the people in the academic community who had been supportive of me earlier seemed to forget who I was. In contrast, distinguished professors Bob Reid from the Massachusetts Institute of Technology and Keith Gubbins from Cornell wrote unsolicited letters to the university president protesting the tenure decision. In the end, I wound up with five job offers, and I chose NC State because I liked the faculty and the direction in which the head, Hal Hopfenberg, was taking the department. The move to North Carolina had minimal impact on my children (the schools and community are great), but it did take a toll on Tom and ultimately on our relationship. Instead of seeking a job in North Carolina, he decided to work full time on the stepper motor controller business that he had been pursuing in his spare time. This turned out to be tougher for him than anticipated. He eventually sold that business and went to work at a small engineering firm in the Research Triangle area.

In hindsight, being denied tenure at Princeton was not all bad; it had a positive impact on my drive and ambition. I had been a hard worker at Princeton, but underneath it all, I hadn't felt like I was competing against anybody. I just needed to do great work. However, after being denied tenure, I felt I had to prove that they made a mistake. This kind of motivation was new for me. I felt misjudged and angry, and this fueled my work. I would show them! As time went on, I realized that I was even more capable and creative than I had thought. Eventually (maybe five years later), the anger went away, but the ambition and enhanced passion for research stayed. Ten years later, I was invited to give a seminar in Princeton's Chemical Engineering Department by my good friend and former colleague Pablo Debenedetti (we had overlapped for six months). I got a chance to converse with my former colleagues, including Bill Schowalter and Professor Y. Bill told me that he regretted the department's decision and had come to realize that it was a mistake; I told him that I forgave them and that it had turned out to be a good thing for me. I even forgave Professor Y, whose disparaging remarks had been so demoralizing to me at the time. He had clearly changed and volunteered that he wished he had done better. Shortly thereafter, I was invited to serve on the department's advisory council. I enjoyed that assignment enormously.

NORTH CAROLINA STATE

NC State has been a breath of fresh air. The Chemical Engineering Department was, and still is, an exceptionally collegial department. My faculty colleagues accepted me from the start and seemed comfortable with my physics background. I became "one of them" as soon as I arrived. There were a few exceptions at first, but those relationships improved over time. The all-female support staff were particularly kind and taught me the basics of Southern manners. I loved when they called me Miss Carol (**Figures 8** and **9**).

At NC State, I began a new chapter in my research: development of equations of state for chain-like molecules, a project that was mainstream chemical engineering but was amenable to a statistical mechanics approach. The keys to the success of that project were Ron Dickman, a very talented postdoc trained in physics, and Kevin Honnell, a Princeton grad student who came with me to North Carolina to complete his PhD. Ron came up with a clever way to construct an

Figure 8

Hall's favorite undergraduate thermodynamics class, Spring 2017.

Figure 9

North Carolina State University Faculty, 2018.

all-purpose equation of state for systems of chain-like molecules such as alkanes and polymers: Generalize the probabilistic assumptions underlying the Flory and Flory–Huggins lattice theories to flexible chain-like molecules moving in continuous space (19). The resulting equation of state was in excellent agreement with Monte Carlo simulations of flexible hard chains. Kevin took that ball and ran with it. His idea was that equations of state for chain-like molecules could be assembled by judiciously combining the equations of state for the segments (e.g., monomers) and groups of segments (e.g., dimers) along the chain (20). This fundamental idea was considered a major leap forward at the time. Prior to that work, most equation-of-state development in the chemical engineering community was based on a semiempirical approach, as researchers tried to add terms to the famous van der Waals equation of state that would do a better job of matching experimental data. Over the next decade, we extended the generalized Flory dimer (GFD) ideas to more complex fluids, devising equations of state for polymer solutions, melts, and blends (21, 22). Grad student Arun Yethiraj (now at the University of Wisconsin) performed simulations and developed integral equations for a variety of chain fluids in bulk and at surfaces (23, 24). GFD's main competition (very friendly, I might add) was the statistical associating fluid theory (SAFT) equation of state developed by Keith Gubbins and his associates Walter Chapman, George Jackson, and Mac Radosz (25). The SAFT people continued developing and refining their equation of state long after we stopped working on GFD, making SAFT a superb state-of-the-art correlation for the properties of all kinds of industrial fluids. Should I have tried to push GFD to be practical as Keith's associates did? I don't think so—that was not interesting to me. We each have to go with our strengths.

In the late 1990s, I turned my attention to much more complex chain-like molecules: proteins. There were two reasons for this move. The first is that to me proteins are just very complex and interesting chain-like molecules. The second is that protein aggregation is a cause or associated symptom of Pick's disease, which led to the death of my father in 1987, and of Alzheimer's disease, which may have caused the dementia that my mother experienced toward the end of her life. Indeed, assembly of normally soluble proteins into ordered aggregates, called amyloid fibrils, is a cause or associated symptom of more than 40 human disorders, including Alzheimer's, Parkinson's, and the prion diseases (26). Another sign that it was time for me to get into biology (my last biology course was in ninth grade) was a prediction that appeared in a fortune cookie: "You will succeed in medical research." Why not?

And then Hung Nguyen, another strong graduate student with a can-do attitude, came along. He developed PRIME, a moderately coarse-grained (four spheres per residue) model of protein geometry and energetics for use with the very fast discontinuous molecular dynamics simulation technique. This allowed us to simulate the spontaneous formation of fibrillar structures in a system containing 96 16-residue polyalanine peptides in approximately 60 h on a fast computer—orders of magnitude quicker than atomic-level simulations (27). [Polyalanine had been found experimentally to form fibrils in test tubes (28).] This was a major breakthrough. Although progress toward understanding the molecular-level mechanisms driving protein aggregation had been made via experiments on particular proteins, studies of fibril assembly based on traditional atomic–level techniques, which follow the motions of every atom on every protein, were impossible because of the long aggregation timescales (microseconds to milliseconds) involved. Later, a talented postdoc, Mookyung Cheon, expanded PRIME to become PRIME20, a protein force field with a unique description of each of the 20 possible amino acids (29). This allows us to simulate the fibrilization of specific peptides (30–32). Recent work with grad student Yiming Wang, Leeds University theorist Stefan Auer, and experimentalists Sheena Radford and Andy Wilson has allowed us to calculate, for the first time, a truly equilibrium phase diagram for a system of peptides, in this case a fragment of the Alzheimer's peptide A-beta (also called beta amyloid) (33). Our simulation-based work on peptide aggregation is starting to be accepted by the protein aggregation community, which is populated almost entirely by experimentalists. Hopefully, our research can help them come up with therapeutic strategies to combat protein aggregation diseases like Alzheimer's and Parkinson's.

A recent research interest of mine is computational protein design. I got into this area when a friend, Paul Agris, formerly of the NC State Biochemistry Department, asked if I could design peptides that bind to specific targets. His goal was to design a peptide that could mimic the ability of the HIV protein, NCp7, to bind to the human anticodon stem and loop (ASL) and thereby block HIV replication. Fortunately, I had a very smart postdoc, Xingqing Xiao, who knew how to make the computer sing. Xiao developed a Monte Carlo algorithm that searches through tens of thousands of peptide sequences to discover those that bind more strongly to a target biomolecule than a known peptide ligand, the "initial guess" peptide (in this case, the peptide discovered via phage display) (34). We used this approach to identify a peptide binder to human ASL with a binding affinity that is 10 times higher than the original phage-display peptide identified by Agris (35). This discovery resulted in my first and so far only patent. Not bad for a physicist, right? Since then, in collaboration with Peter Mirau and Rajesh Naik at the Air Force Research Laboratory, we have designed a peptide that recognizes a biomarker for heart attacks, cardiac troponin I; the level of detection achieved is better than that of the high-sensitivity commercial assays that require a clinical lab and 24 hours to develop (36). More recently, along with my young NC State colleague Stefano Menegatti, we designed a peptide that shows promise for becoming a synthetic mimic for protein A, the workhorse ligand that is used in industry for monoclonal antibody purification. This is a whole new world for me—fascinating!

Figure 10

Hall group reunion at the American Institute of Chemical Engineers annual meeting, Fall 2016.

CONCLUSION

As you can see, my research interests and approaches have evolved over time to become more down-to-earth and practical. I seem to be even more excited about doing research now than I was earlier in my career (**Figure 10**). One of the things that makes it so much fun is working with nice and smart people and discovering new ideas and thinking up new ways to do things together. I have had the pleasure of working with some great students and postdocs. A major ongoing concern for me, and for most of the research community, is funding, which has gotten much harder in recent years. So, I am trying harder (and hopefully smarter). Wish me luck! I have been asked when I will retire. My plan is to continue working as long as my health, energy, brainpower, and ability to do my job effectively hold out.

Young women that I meet have asked how I cared for my children while working full time, and how that affected them, me, and my work. The answer is that Tom and I hired nannies to take care of the children in the daytime, and we took care of them the rest of the time. When I was at home, my focus was on my children, and when I was at work, my focus was on my work. This seemed natural to me; it never occurred to me to stop work to raise my children. I do remember a now-famous professor who visited Princeton when I was pregnant with Adam asking me who was going to raise my child. (In those days, most mothers stayed at home.) In retrospect, I and my children feel I did the right thing. I asked. Katie, Adam, and Norah turned out just fine.

Figure 11

Hall and Newman families together at the beach, 2018.

Life of course has its ups and downs. I have had some tough times since coming to NC State. In 2001, I was diagnosed with breast cancer and underwent treatment for about nine months. In 2006, Tom and I separated, and in 2009, we divorced. That was a difficult time for me, but I eventually concluded that it was for the best. After a period of adjustment, I started to date using online services like Match.com. This was, in many ways, hilarious; I could write a book about those times titled, *Dating after 60: A Comedy*. In September 2011, on Erev Rosh Hashanah, the evening before the start of the Jewish New Year, I met my partner, Sheldon (Shelley) Newman, a widower trained in electrical engineering who lights up my life. Shelley has been the CEO of some large health-care companies, is still working, and is comfortable with me being me. My three wonderful children—Katie (a singer in New York City), Adam (an artist in New Orleans), and Norah (a teacher in Raleigh)—are making their way through life, and my three fine grandchildren make me smile. Life is good for now, and I am grateful (**Figures 11** and **12**).

My professional and personal lives have been enormously enriched by my interactions with various people in the community. At NC State, I have had a long research collaboration with Orlin Velev on colloidal particles and with Jan Genzer, Saad Khan, and Benny Freeman on polymer materials. My research interactions with my former students and postdocs who are now academics—Aysa Akad, Ronald Dickman, David Faux, Daniel Forciniti, Alice Gast, Barbara Hacker, Arthi Jayaraman, Monica Lamm, Harry Ploehn, Christine Soteros, Andrew Schultz, Qing Shao, Arun Yethiraj, and Yaoqi Zhou—were particularly rewarding. I have also enjoyed research collaborations with colleagues elsewhere, including Martin Cohen-Stuart, Marc Donohue, Amparo Galindo, Gregory Hudalla, George Jackson, Sabine Klapp, Maria Kula, Raquel Lieberman, Anant Paravastu, Ted Randolph, Martin Schoen, and Yara Yingling. I am fortunate to have had the

Figure 12

Sheldon Newman and Carol Hall, 2017.

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What message do I want to convey to young people? That even though I started out with no particular direction, I did some things right. I kept an open mind, took some risks, was not quick to close doors, allowed myself to fall in love with research, didn't stay down for too long, and was open to new ideas, new opportunities, and new friendships. It helps to be passionate about what you do, and to have a sense of fun when you can.

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Errata

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