Biography of Barbara J. Garrison

Barbara Jane Garrison was born in Big Rapids, Michigan, on March 7, 1949. After serving as a medic in World War II, Barbara's father Homer "Gary" Garrison had resumed his education at Ferris State College at the instigation of his wife, Elizabeth "Bettie" Steinberg, Barbara's mother. Gary, son of a Michigan family in which children traditionally did not go to school beyond the eighth grade, was the first in the Garrison family to go to college and he graduated in Pharmacy. Bettie, daughter of a clerk in a dry goods store, grew up in a small town in Missouri and studied with her sisters in Long Beach, California. She met Gary while she was working at Fort Leonard Wood and married him right after the war, in 1945. When Gary graduated in 1951, the family moved to Lansing, where Barbara's sister Cindy was born two years later. Barbara's parents, like generations before them, decided that the opportunities were greater in the West. So, in spring 1956 they moved to Phoenix, Arizona. They still reside in Scottsdale today, also home to Frank Lloyd Wright's Foundation, Taliesin West.

The Formative Years

Barbara's father encouraged her to enjoy math and physics. At an early age, he taught her cribbage. Even though she remembers helping him at doing repair works, apparently, it did not rub off to make her an experimentalist! Barbara's mother, who was in the fife and drum core in high school, encouraged her to take up clarinet, which she played for eight years.

In grade school, she marched with the band in the annual Rodeo parade, played softball, and was in the Brownies and Girl Scouts with her mother as a troop leader. At one of their meetings, she was introduced to genealogy, a discipline to which she would remain hooked for the rest of her life. In eighth grade, she learned how to use the slide rule. She was arguing with her teacher about why a negative number times a negative number is positive: "He kept making an analogy to a movie projector going in reverse and then reversing itself. Didn't make sense to me and as I later found out is not the right answer". Years later, her parents told her that her eighth grade math teacher told them that she knew more math than he did!

In 1963, Barbara went to Camelback High School, a large school with about 3000 students for the four years. In freshman math class, she remembers this sad November day, when a math teacher came to announce the death of John Fitzgerald Kennedy. Barbara continued with the band until her senior years but when it became a choice of band or physics, she took physics. She graduated in 1967, fourth out of 600−700 students.

After high school, Barbara applied to the Arizona State University and the University of Arizona, mostly because the finances of the family would not have allowed her to study in another state. The Arizona State University granted her a scholarship, so she went and majored in physics. She got active in clubs and was in an honor society in both her junior and senior year. She loved living in a dorm and being on her own. Her best friend and room-mate in much of college was Barbara Grant. They were $(BG)^2$! Grant encouraged her in classes and the activities. Some of her favorite classes concerned mathematical methods of relevance to physical sciences. She still remembers the elegance of the orthogonal polynomial such as Hermite, Legendre, and Chebyshev. The mandatory general education classes in Impressionist to Modern Art and Intro to Architecture have stayed with her throughout her life, too. "As an advisor, I have encouraged my advisees to appreciate the general education classes as a result of this experience".

Since the undergraduate quantum physics instructor at Arizona State had a poor reputation as a teacher, Barbara revolted and chose to take quantum mechanics in the chemistry department from Professor Sheng (S.H.) Lin. Sheng Lin was one of the most distinguished members of the ASU faculty and later returned, along with many other Taiwanese including Nobelist Yuan T. Lee, to the Academia Sinica in Taipei. Sheng encouraged Barbara and arranged for her to work with another faculty member the following summer, doing semiempirical

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electronic structure calculations. "This is when I started leaning towards being a chemist."

In the summer of 1971, Barbara graduated summa cum laude from the Arizona State University.

From Physics to Chemistry and...Surface Science

Barbara arrived at Berkeley in September 1971 as a Ph.D. student in physics. She did well in the two classic first year physics courses, graduate electromagnetism with Dave Jackson and graduate quantum mechanics. However, along the way, Barbara decided her passion was for the physics of molecules, a discipline more typically included in chemistry departments in North America. Accordingly, she decided to transfer from physics to the Ph.D. program in chemistry. Brad Moore was the Assistant Chair of Chemistry, and cheerfully made this transfer pretty easy for Barbara. Her penance was to take two lab-free organic chemistry courses, plus Ken Pitzer's course in thermodynamics.

Henry F. Schaefer III: "Undoubtedly because of our good looks, Barbara signed on with two assistant professors in the chemistry department at Berkeley, namely Bill Miller and me. She initially worked with Bill and me on the Penning Ionization of triplet metastable helium atoms, resulting in her first paper (1973). Barbara's only sole paper with me (I doubt she even remembers it) involved the lowest triplet and first excited singlet states of formaldehyde."

She did publish a paper with the late Charlie Bender and Henry F. Schaefer III that had significant impact. This was the prediction, in 1975, that the barrier height for the degenerate H + FH → FH + F reaction was very high, about 40 kcal/mol. Although Dudley Herschbach and others strongly objected to this prediction on intuitive grounds, they were eventually vindicated by the definitive experiments of John Polanyi (1978).

On a fateful day, the Lawrence Berkeley Laboratory informed Barbara's advisors that they could no longer use the CDC 7600 for their research, unless they could pay $1000 per hour for computing time. Since they had no other computing resources, this was a major challenge. In addition to her other dynamics projects with Bill Miller, Barbara had developed a taste for the quantum dynamics of inelastic collisions. Since Bill Lester at the IBM Research Laboratory was a good friend and the worldwide leader of research in nonreactive chemical dynamics, Barbara began commuting to IBM in San Jose. This 50 mile commute was made the more wearisome by the difficulty in procuring gasoline during the first energy crisis. Henry F. Schaefer III remained involved, contributing to Barbara's two papers on the potential energy hypersurface for $He-H_2CO$. Per Siegbahn, a Miller Fellow postdoc with Schaefer at the time, was also involved.

Henry F. Schaefer III: "From the very beginning she had a lot of chutzpah! If 1971 was an era in which women were to be quiet and subservient, nobody had ever effectively conveyed this information to Barbara. Having since directed another 100 Ph.D. students, I can place Barbara's audacity in a broader context. When one first meets a new graduate student and encounters seeming impertinence, it is important to discover if there is genuine scientific substance behind it. If the answer is 'yes', as it most certainly was with Barbara, some outstanding science can happen. When the answer is 'no', I encourage the student to move on to greener pastures. One of the most refreshing features of Barbara's personality is that she pays no false compliments. For these and other reasons, Barbara is one of my most cherished former Ph.D. students."

Barbara made several friends in graduate school whom she still sees at meetings or interacts with professionally, including Steve O'Neil, David Yarkony, Cliff Dykstra, Bruce Garrett, Sally Chapman, John Adams, David Oxtoby, Charlie Bauschlicher, Gretchen Schwenzer, and her room-mate for several years, Karen Ho. "Living in Berkeley was great for me. My high school and college were effectively segregated. Berkeley introduced me to a large diversity of ethnic groups include the crazy people of Telegraph Avenue."

She graduated from Berkeley in 1975, with a thesis entitled "Cooling of Interstellar Formaldehyde by Collision with Helium: an Accurate Quantum Mechanical Calculation".

At the end of her graduate years, Barbara felt she needed something different and looked to the emerging area of surface science. She took a postdoc with Steve Adelman at Purdue University. While at Purdue, she made an encounter that would seriously impact on the rest of her life.

Nick Winograd: "We met in the fall of 1975 at Purdue shortly after she arrived on campus to do a postdoc with a theoretical chemist. I was going through a divorce, and we were casual friends for a few months talking science a bit, before our relationship got serious. Her research was going well, but the postdoc experience was rather stormy."

A number of people Barbara and Nick met at Purdue became their lifelong friends.

Peter Kissinger: "As graduate students in the late 60's, we took our 'vow of poverty' and learned to seek food as sustenance for laboratory work. This habit we continued as postdocs and then as junior faculty. At Purdue in the late 70s I discovered that theoretical chemists could actually cook and would do so in lieu of laboratory experiments. I made a deal with postdoc Barbara and Assistant Professor Nick that if they would both cook, I would do the dishes. We all won and celebrated with a glass of wine of questionable quality."

Frank K. Fong: "At that time, a group of us young chemistry faculty members would carry on a weekly ritual of getting together at the close of business on Friday, each taking turns hosting the others for cocktails and, then, dinner at a favorite restaurant. Of this group, Nick Winograd, Dennis Diestler and I formed the nucleus, later joined by Barbara. [.. .] Through our Friday gatherings and scientific talk, Barbara, Nick and I became fast friends. But soon I became diminished in the three-way interaction as the odd person out, even while their relationship ripened into romance."

During her second year at Purdue, Nick, Graham Cooks, and Nick Delgass decided to get an instrument for secondary ion mass spectrometry (SIMS). Nick asked Barbara to explain the significance of the clusters emitted under ion bombardment of metallic surfaces. Did it imply that the atoms were adjacent to each other on the surface?

In 1976, Barbara and Nick visited Drew Evans and Peter Williams, at the University of Illinois, where Drew was director of their surface analysis facility. It was a key visit for both of them. Nick had won a Guggenheim fellowship and planned to sit in Dave Shirley's lab at Lawrence Berkeley Lab during the 1977−78 academic year. Since Barbara was a Berkeley grad, they arranged for her to assist in the freshman chemistry program. She was a bit discouraged, because the postdoc was not going very well and was seriously considering other career options. Drew Evans suggested that they hook up with Don Harrison at the Naval Postgraduate School, about 75 miles south of Berkeley in Monterey, California. He noted that Don Harrison was trying to make computer simulations work using overnight runs on an administrative IBM computer using punch card input.

Don was modeling the sputtering event with molecular dynamics simulations but his work was not having the impact that Drew thought it should. He thought that with Barbara's theory expertise and Nick's interest in surface chemistry, the three of them could have a productive interaction. So, in 1977, Barbara and Nick trucked out to Berkeley and started working with Don Harrison.

Nick Winograd: "Don was a bit of a curmudgeon. Barbara was a stickler for high standards, so the two of them made quite a pair. My role was to keep them thinking about the right calculations, and to stop any violence. The system at the Postgraduate school was not ideal. Don could have use of the computer for overnight, but not much got done. Our first calculations used 128 Cu atoms and it took days."

Echoing Nick's earlier thoughts, Barbara and her new accomplices tackled for the first time the question of cluster emission, crucial for the nascent SIMS method, in the article "Formation of Small Metal Clusters by Ion Bombardment of Single Crystal Surfaces". The article was coauthored by Nick and Don Harrison and issued in August 1978. They showed that small clusters with $n > 7$ do not eject as intact parts of the solid but rather form in a region right above the surface. It was this era where they switched from using punch cards to submit a computer job to using a 300 baud teletype machine.

Barbara and Nick started to enjoy the southern California coast. They spent several days in Big Sur with their cat, got to know all the restaurants in Carmel and Monterey, and started to become very good friends with Don Harrison and his wife, India, spending time and attending plays together. At the same time, Dave Shirley generously gave them access to the supercomputer at Lawrence Berkeley Laboratory, which was at least 10 times faster. There, with the help of the excellent graphics group of LBL, they made their first sputtering movies. In those days, the movies were made by microfiche technology, where each frame was printed to 16 mm film. Barbara and Nick's contributions to this effort were to bring some chemical interest to the problem, secondary ion mass spectrometry, and to try to make the calculations bigger and more rigorous. Don Harrison provided the basic molecular dynamics (MD) code, remnants of which are still in today's working code.

Nick Winograd: "There was one instance that typifies the year. Barbara and I were headed to Sequoia National Park and planned to stop off at Don's place to start a weekend job running. I helped set up the data set at the punch card machine. We were looking at the effect of angle of incidence. About half way to the park, Barbara realized that we had made a terrible error. The angles were supposed to be input as the cosines of the angle, rather than the angle itself to save computer time. We forgot about that little Harrison maneuver. So, we turned around, drove all the way back to Monterey and resubmitted the cards before finally starting the weekend. The whole year was like that, an intense mix of work and having a good time."

Her scientific production got boosted by the collaboration with Don Harrison and Nick. There were between 10 and 15 papers that were published as a direct result of the work they did that year. Don Harrison remained revitalized until his premature death in 1988. Barbara shed her interest in changing careers, deciding maybe she had a future in academics.

On April 19th, 1978, Barbara and Nick got married at the Alameda County Courthouse in Oakland California. They took their honeymoon at Alcatraz. Shortly after, she marched back to Purdue after their sabbatical year in search of a tenure-track faculty position.

The next years were intense. Barbara was hired as a visiting faculty member at Purdue for 1978−79. She developed many close friends at Purdue: too many to name, but also a few who were not so friendly. The research continued with Don Harrison, long distance, and the papers continued to appear, giving her a significant national presence. When Penn State came knocking with two job offers, she convinced Nick that the best thing for both of them was to move on. Although he found it difficult to leave Purdue, he recognizes that it turned out to be one of the best career moves in his life.

Dennis J. Diestler: "I expended a good deal of effort to persuade my Purdue colleagues to keep Nick and Barb at Purdue after they had received the Penn State offer. It was my one, and only, reluctant foray into the arena of academic politics, at which I am singularly incompetent."

Pete Kissinger: "Allowing their escape to Penn State was a grave error on Purdue's part, but their ongoing collaborations have done much for science. At least we have them back in the Big Ten and still cooking."

Frank K. Fong: "The months after Penn State made the bids for Barbara and Nick were stormy. [.. .] Although Barbara developed many close friendships at Purdue—too many to name, she also ruffled the feathers of a number of our colleagues in the physical division. And, despite my strong push at the provost level to promote Nick to full professor at once, Haas was unable to fire up the dean to counter Penn State's offer. The department opened up a new position in "theoretical analytical chemistry", but did no more. Nick tells me that it was Barbara, not he, who made the decision to leave Purdue. As much as I bemoaned the loss, I was in full accord with that decision. The meteoric rise since in their respective careers would prove it correct."

The Penn State Years

In 1979, Barbara and Nick moved to State College, PA, where she took her appointment as an Assistant Professor at the Chemistry Department of the Pennsylvania State University. The first years at Penn State were terrific for both of them. They got new grant money and IBM provided Barbara with a mainframe computer that was identical to the one associated with the University. The relationships Barbara built with the Center for Academic Computing during 1980 still serve her well today.

With her new resources Barbara continued to develop her simulations of the sputtering process with various systems including metal crystals, rare gas, but also atomic and molecular overlayers. Two of the important questions she tackled over those years concerned the determination of surface structure and, already, the emission of intact organic molecules using keV ion beams. Her publication list flourished with about 30 articles out over the first five Penn State years. Her first paper in *Science* "Ion Beam Spectroscopy of Solids and Surfaces", cowritten with Nick, came out in 1982, just to mention that one. Nick's role in the MD calculations, however, would rapidly diminish because of his new responsibilities as head of a lab.

In 1983, Barbara received a phone call from Dr. R. Srinivasan, a pre-eminent photochemist at IBM Yorktown. He had seen results from her sputtering simulations and invited her to visit IBM and discuss modeling ablative photodecomposition, a phenomenon he had recently discovered. They put together a simple MD simulation to explain the system. As we will see, her interest in this phenomenon would rejuvenate later.

Barbara and Nick took a second sabbatical in 1985−86 at CalTech. Barbara sat in Bill Goddard's lab, and Nick interacted with Tom Tombrello. During that period, they worked particu-

larly hard at finding better interaction potentials for the MD calculations. Because the quality of the experimental energy and angle distributions from single crystal metal surfaces produced by Nick was much improved, it was more challenging to see how close the models could come to the data. To obtain more reliable theoretical results, Barbara adopted a many-body embedded atom approach to the problem. The success of these calculations led her on to even better descriptions of the energy dissipation, and the inclusion of organic molecules on surfaces became more realistic.

Nick Winograd: "Home computing was just beginning to take off. We had a condo near CalTech, along with some of the first practical PCs that could logon to mainframes. Using modems, many of these calculations were done at the Penn State facilities, quite an accomplishment for those days. The big PC with its flat top provided a warm sleeping place for our two cats."

Barbara's first grad student, Don Brenner, was modeling silicon molecular beam epitaxy, a project that would last about a decade and produce many articles. Their effort enabled modeling of an increasingly broad variety of low energy reactive processes at surfaces. During his Ph.D. period, Don got his start in developing potentials, a Si one, while Barbara was on sabbatical at CalTech. Her interest in modeling reactions continued with another graduate student, Tracy Schoolcraft. In 1991, they published the first study on modeling etching reactions of Si due to interaction with F, using the Stillinger−Weber potential, in *The Journal of American Chemical Society*.

Barbara and Nick became good friends with their Penn State colleagues Steve and Pat Benkovic. During these years, the four of them took vacations to Kenya and Virgin Gorda. But a common interest in biking led to almost annual biking vacations to France. They hit most of the major spots: Loire, Burgundy and Provence, and the experience left Barbara with a great appreciation for fine food and wine, something that continues to strain their budget to this day!

Over the years, Barbara got seriously involved in the University committees, such as the University Promotion and Tenure committee. In 1988 the Dean chose Greg Geoffroy to be Department Head. Within 11 months, Geoffroy became Dean of the College of Science and, as a result, Barbara became Department Head at age 40!

Henry F. Schaefer III: "I am proud not only of her outstanding research, but also that Barbara was the first woman in the U.S.A. to be the Chair of a major university chemistry department."

Mark Maroncelli: "Barbara is now on her second round as department head, once when she was unusually young for the position and again just last summer. In my opinion she does a terrific job in this largely thankless role for a number of reasons. Barbara loves organizing; she truly enjoys supervising and mentoring people and she revels in big projects like construction of the new chemistry building. I credit the success of the department's new home to her careful stewardship of its design, a project she took on between her two terms as department head. As Head, Barbara isn't afraid to dig into the details of a problem herself but is also good at delegating responsibility. She's not afraid to make unpopular decisions when necessary and especially in her first stint as department head, Barbara ruffled a few feathers. But she has always had the best interests of the department in mind and she works tirelessly to see that we move forward. Even the ruffled realize her commitment, and that's why she was recently asked to lead the department once again."

Also, as several of Barbara's friends and colleagues remember, establishing such a successful scientific and academic career as a woman was neither common nor easy.

Pete Kissinger: "It was a very sorry state back then that women in science were not appropriately recognized and/or appreciated by those of either sex. The culture is still improving in this respect, but the rate constants for cultural change are no doubt very slow...a 20 year half life is not unusual." However, with her usual sense of confidence and a decidedly positive outlook, Barbara somewhat counters the argument today: "Although we claim at times that women were discriminated against, being a woman often opened doors. I got to be involved in lots of activities at a national level because of being a female department head".

Whatever the exacts reasons were, she was, over the years, in advisory and review panels for the National Science Foundation and the Department of Energy, on the Governing Board of the Council for Chemical Research and on the Board of Chemical Sciences and Technology, a committee of the National Academy of Sciences. She also did external reviews for nine chemistry departments.

Scientifically, her focus was more and more on modeling reactions on surfaces. Deepak Srivastava was modeling molecular beam epitaxy at silicon surfaces and developing Monte Carlo methods for longer time processes, while Ramona Taylor incorporated the Brenner hydrocarbon potential into the sputtering code and did the first simulations of sputtering of organics that accounted for chemical reactions. They showed that H abstraction and other reactions between molecules are possible consequences of the bombardment by energetic projectiles. Eric Dawnkaski modeled diamond film growth with kinetic Monte Carlo and molecular dynamics approaches. One important result, published in Science in 1992, was the insertion reaction of carbon at the diamond surface. Dave Sanders, who was in the group as a postdoc, overhauled the several sputtering codes and combined them into one single code that is still used and developed today by Barbara's co-workers and many collaborators around the world. It is also during that period that a future long time collaborator, Zbigniew Postawa, would make his appearance in Barbara's life, first as a one-year visitor in Nick's laboratory.

A Builder

Back then, Barbara and Nick lived three miles from campus, with a line-of-sight from the chemistry building to their roof. And, they already had high speed Internet to the house! With a microwave link, they had excellent access in an era when people were using 1200 and 9600 baud modems: "Pretty cool. Two of our neighbors borrowed the signal." This was the era before one started to worry about security.

Geri Richmond: "I always know when I see Barbara that she will show me some gadget or fad that I've never seen or heard of before - such as the portable phone in her office back in the 80s when everyone else's phones were still tethered to the wall. Or the lighting system in their house that could be completely controlled by a panel of switches next to her bed - while the rest of us are schlepping around our house in our slippers trying to turn off every individual light in the house before retiring. And while the rest of us were in our middle age physical exercise ruts, she got a physical trainer (coach) and started into some deep massage therapy treatment."

In the early nineties, the couple bought a 56 acre piece of land, some 18 miles east of Penn State. They would soon have their new estate built there, overlooking the surrounding fields, with the rolling Central Pennsylvania hills as a backdrop and their own private driveway meandering through the woods..."Chemistry Lane"!

In 1995, Leonid Zhigilei joined the group as a postdoc. With his help, Barbara resumed the thread started in the eighties with her seminal attempts into modeling laser-induced processes with R. Srinivasan. Leo developed the breathing sphere model for laser ablation, which was published in 1997. A graduate student, Yara Yingling helped Leo and Barbara by developing the methodology of including chemical reactions in coarse grained simulations. Arnaud Delcorte joined in 1999, starting another long-standing collaboration that would be pursued into his next appointment as a professor in Belgium. In fact, this was the era when many of Barbara's collaborations were formed or cemented, for instance, with Zbigniew Postawa in Cracow, John Vickerman in Manchester, Andreas Wucher now in Duisburg-Essen, Kristin Krantzman in Charleston and Roger Webb in Surrey. Tracy Schoolcraft also came back for a sabbatical in 1999/2000. Barbara's "computational chemistry" group hosted the International Conference on Simulations of Radiations in Solids (COSIRES) at Penn State. The diversity of the research projects and active interactions with collaborators provided fertile ground for education and professional growth of students and postdoctoral researchers in Barbara's group.

Leonid Zhigilei: "The time I spent in Barbara's group was highly rewarding for me and the experience I got had a strong impact on my future carrier. Barbara's approach to research work combined the rigor and attention to details with keeping sight of the "big picture" and the connections between the computational predictions and the intuitive understanding of the physical phenomena. The discussions at the weekly group meetings, along with occasional joint meetings with Winograd's group, covered a broad range of computational techniques and scientific topics and provided me with ample of opportunities for learning and exploration of new ideas. I 'copied' some of the traditions of Barbara's group when I started my own group at the University of Virginia."

Tracy Schoolcraft: "I was Barbara's second Ph.D. student at PSU during the late 80's and she was my first female science professor. When I think of those days, I think of backing up the computer with reel-to-reel and 'computers' that only did word processing. We were in Davey lab. She supplied us with fresh roasted coffee beans from The Cheese Shoppe and thus I learned to love black coffee. (Matter of fact, I still get their coffee shipped to me regularly.) I later returned to do my sabbatical with her, this time in Whitmore. She taught me how to write journal articles, present posters and oral presentations at conferences, review and write grants, at a time when only a few graduate students got these kinds of experiences. I know I tried her patience, like taking until the very last cumulative exam to pass the required six! With Barbara, you get good, straightforward feedback and it was up to you to use it. I greatly appreciate the help and level-headed advice she has given me after graduation; making the transition to life-after-the-Ph.D. has its challenges. I feel very fortunate to have Barbara as a mentor and role model and I look forward to more years of advice."

In 1995, following several years of visiting their country estate during the weekend biking rides, Nick and Barbara started to build a new house in Spring Mills. The architectural design of the new house and the surrounding garden was strongly affected by Barbara's taste. After completion in 1996, the house became the site of the annual group parties and has been admired by friends of Barbara and Nick who enjoyed their hospitality.

Frank K. Fong: "My wife Margareta and I have been frequent guests at their palatial home on Chemistry Lane near the Penn State campus. Nearly 10,000 sq. ft in area, the Garrison-Winograd mansion has only one guest room in addition to the master bedroom. There they house us in the guest suite overlooking a vast expanse of manicured gardens, surrounded by the beautiful Pennsylvania landscape of hills and dales."

Geri Richmond: "I have always admired her ability to work hard and play hard. We all know how hard she works and her commitment to science - but she balances this with her wonderful country estate, complete with a full garden and wonderful places to sit and watch the countryside and fish in their pond."

At a time when she was watching her new house get built in 1995, Barbara was appointed Chair of the New Chemistry Building committee by Penn State. She thoroughly enjoyed working with the architects, the other design professionals, and her colleagues in planning, designing, and constructing the new building. The building would emerge from the ground and be ready for occupation in 2004.

Mark Maroncelli: "Barbara worked tirelessly chairing the building committee. She clearly loved this job, which gave her a chance to build something else from the ground up in addition to her home. I don't know how buildings like this one typically go but it is my impression that we've been about as trouble-free as one could expect, and the space is really beautiful."

Arnaud Delcorte: "Barbara has a genuine interest and excellent taste for art in general and architecture in particular. It already struck me as I was taking my first steps as a freshly appointed postdoc in her offices at the old Whitmore Building. First thing you would see after passing the door was a small white wall with a colorful abstract painting, then turning around that wall, you'd enter a vast lobby with comfortable chairs and a coffee table, two aisles with offices were developing symmetrically from this immaculate and perfectly lit foyer. Then I discovered her beautiful mansion in Spring Mills, that immediately reminded me of the "honeycomb" (Hanna) house of Frank Lloyd Wright, who we both admire. A perfect architecture for the land they acquired. Later on she happily carried an even more ambitious architectural project, with the new chemistry building. I think that interest springs from her profound need to organize the world around her in a way that is not only rationally appeasing, but also pleasing to her eye...and ours!"

Not only interested in making buildings break ground, Barbara was also getting more and more knowledgeable about her roots, as a human being, through the study of genealogy and the reconstitution of her family tree.

Frank K. Fong: "There are a few things casual friends of Barbara probably do not know, like what her great granduncle, Walter Hinton, did as a young man. Hinton was the pilot of the Curtiss NC flying boat 'NC-4', the first aircraft to make a transatlantic flight in 1919, eight years before Lindbergh's. On one of my recent visits, she showed me a little booklet she wrote, a fictionalized account of her great grandfather's immigration to the U.S. from Germany."

At the turn of the new millennium, Maggie and George, Barbara's beloved cats, had joined the Garrison family in Spring Mills.

World Citizen

The next and most recent period would find Barbara with her largest group ever, in the years 2004−2008, and a lot of activity in both the sputtering and the laser ablation areas. The ablation model underwent new developments, with the introduction of realistic chemical reaction schemes, so the irradiation effects induced in complex molecular samples, such as amor-

phous polymethyl methacrylate, could be described. On the side, she also moved into describing dissolution of minerals in water.

At the same time, she had with her a strong extended group of collaborators from other states and countries, forging ahead in a concerted way. The regular visits of Zbigniew Postawa over the years helped Barbara supervise the group and direct it at a time when secondary ion mass spectrometry was going through a quite interesting mutation, with the introduction of clusters and molecules as routine projectiles for analysis. In 2003, when John Vickerman introduced the first commercial C_{60} gun with Ionoptika, Barbara and Zbigniew's simulations were right on the spot, showing the collective motion of the surface atoms displaced by a fullerene impact and the nanocraters formed at the surface of metals. Similar effects, but larger craters, and subsequent emission of large intact molecules were shown to occur in polymers, through the collaboration with Arnaud Delcorte. The experimentally observed deposition of C_{60}'s carbon atoms in silicon was explained using chemically sound potentials by Kristin Krantzman and first attempts at implementing electronic effects in Barbara's classical model were successfully made by Andreas Wucher.

John Vickerman: "In many ways I think these MD simulations have reached maturity through this work. In early days the simulations followed quite a long way behind experiment, now simulation and experiment are progressing together. The simulations are suggesting new experiments and directions, not just providing insights into experimental observations. It is a measure of Barbara's stature in the field that so many colleagues now count it a privilege to work with her and have her involved in their work."

Leonid Zhigilei: "Barbara's attention to experimental data and focus on explaining experimental observations clearly distinguishes her among the computational scientists I have interacted with. The lack of agreement between the model predictions and experimental results has been one of the main driving forces for the advancement of Barbara's models and, in some cases, complete redesign of the computational approach. Puzzling experimental data occasionally served as a starting point for a new project. This was the case, for example, with modeling of MALDI that started from the discussions between Barbara and experimental colleagues and has motivated the design of a family of coarse-grained models for laser interactions with molecular systems."

At a workshop in Scotland, after two beer sessions with Zbigniew Postawa and her student Mike Russo, they figured out a new scheme to realistically model repetitive bombardment of a surface, a major coup with the parallel emergence of practical molecular depth profiling by fullerene beams. This was April 2007. An image taken from one of the recent simulations constitutes the cover of this special issue.

At the national level, Barbara pursued her activities with the American Chemical Society, as a Program Chair for the Physical Chemistry division in 2005 and as the Division Chair in 2006. In 2009, 20 years after her first appointment in that capacity, she was asked to serve as the Head of the Department of Chemistry again.

Whether biking in the rural south of France, climbing on the Hawaiian volcanoes, jogging in the busy megacities of Asia, sailing in the arctic waters near the Spitsbergen islands, or simply relaxing in the Turkish baths of Istanbul, Barbara always enjoyed traveling and discovering the natural and the human world surrounding her.

In the past few years, Barbara and Nick got in the habit of spending the coldest months of the winter in Manchester, U.K., by their long-time friends John Vickerman and his wife, Linda Watson.

John Vickerman: "Not only have these visits been a real stimulation of our and their work, it has also provided other opportunities for Barbara. She delights in, and has mastered the UK rail system. She knows in detail how to get the best reduced first class rail fares between Manchester and Roger Webb's lab in Guildford and many other places too, particularly those containing a Michelin Star restaurant. [...] Barbara and Linda are now fully into spas and similar experiences. She always shows herself up for a new experience!"

So, what experience is next on Barbara's agenda?

Arnaud Delcorte
Henry F. Schaefer III
Nick Winograd
Leonid Zhigilei

Guest Editors

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