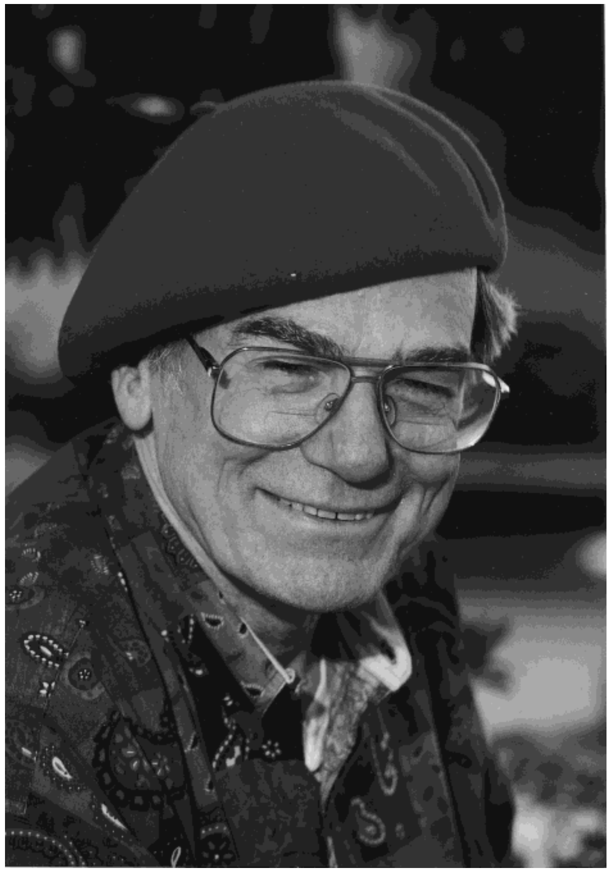

Photograph by Robert Paz

William A. Goddard III

Critical Points and Random Events That Shaped the Early Career of William A. Goddard III

My grandparents all moved to Imperial Valley in the desert of southern California in the period 1905−1912. They came from Arkansas (William Andrew Goddard I; his father Peter was a Baptist minister, his mother Lucy Minor Goddard traced her relatives back through the revolutionary war), Colorado (Frances Thomas Goddard Whitsett; her father was half Comanche), Angelina County in east Texas (Lias Austin Bright; one of his grandmothers was Cherokee), and Coushatta, Louisiana (Lula Gray Bright). Except for the Indian, their ancestors were from Germany, Holland, England, Scotland, and Ireland, arriving in the U.S. in the period from 1700 to 1840. My dad (born in Holtville, California in 1912) left school in 9th grade (his younger siblings were the first in his family to finish high school; none attended college). My mom (born in Calexico, California in 1918) graduated from high school, the only one in her family to do so [she went to college part time in her 50's (while working full time on the night shift at Pacific Telephone), getting a BA in English]. I was born in a small cabin behind the baseball stadium (on the wrong side of El Centro) on March 29, 1937. My dad made the wooden boxes used to ship lettuce, carrots, grapes, and cantaloupes. Consequently, we moved forth and back every year between Imperial Valley (El Centro) and the central (San Juaquin) valley of California [Delano, Mac Farland, Oildale (suburb of Bakersfield), Lodi, Firebaugh, and a few tiny towns that no longer exist]. We also lived once in Yuma, Arizona (the farthest east I had traveled until I had a Ph.D.) and several times in Coachella Valley (Indio, Thermal). We lived in a house trailer that was moved from trailer park to trailer park. Our only books were the bible and a Webster dictionary, but my mother took me to the library (most funded by Carnegie) nearly every Saturday to get books (I liked psychology).

In 1946 Jean Pangle (who managed the Standard Oil service station in El Centro) gave me a book on baseball statistics, and I quickly became an expert on fractions and decimals (calculating batting averages, slugging percentages, earned run averages, win−loss percentages), although I had no idea what a decimal point was. Consequently, from fifth grade on, I was always the top student in arithmetic. My parents never once suggested that homework or school was important, and I generally studied just the things that I found interesting (even then totally undisciplined). In those days, California tracked students (putting the brightest together in one class and the slowest in another), and I was always put in the bright class (despite being considered as an underachiever) while most of the "fruit tramps" (as we were called) were put into the slow class. Since my friends were all middle class, it was natural to plan a college prep course of study in high school. However, my mother thought that going to college was unrealistic and strongly encouraged me to take practical courses. As a result, I took a vocational course each

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year. It turned out that her advice was right. I was an excellent draftsman, and in the summer before my junior year in high school, my drafting teacher (Guy Hatch) was asked by the Imperial County Assessors Office to recommend a draftsman (theirs had been drafted for the Korean war). As a result, I worked half time my last 2 years of high school, full time during summers and vacations, and full time for a year after high school (we stopped moving for my last 2 years of high school), saving the money that allowed me to go to college. As a draftsman, I deciphered the legal descriptions for the farmland in Imperial County and drew maps for the assessors to use in appraising the properties for taxes. In those days I could freehand-print in ink the details on these maps (a lost skill as my students and secretary will attest). This allowed me to save $2200, probably the equivalent of about $8000−$12000 today.

From high school I remember my English teachers in El Centro (Proudfoot and Gillette) and in Delano (Miller) and my math teachers in El Centro (Hinshaw) and Delano (de Fraga) as particularly influential. I also remember my high school physics teacher as an abomination and my chemistry class as stupid. Since I worked immediately after school and all day Saturday, I did little in extracurricular activities except for organizing the chess club. My best friends in high school (Tom Foss and Paul Werve) were going to become engineers, and I decided that I would too. We worked on our motorcycles and automobiles together, taking engines apart and putting them together, tuning the engines, and repairing brakes and clutches.

At the beginning of my junior year in high school, I wrote to get brochures from three colleges. I learned that the annual tuition at Stanford was $750 while Caltech's was $600 and UCLA's was $92. Thus, I knew that I would go to UCLA. I also knew that all UCLA required was B's and A's (plus a high score on a special exam for engineers), which would be easy so that I would not need to study hard. Since I worked after school, I had to ditch class to get haircuts, buy clothes, buy parts for my car and motorcycles, etc. This caused lots of problems with the high school administration, leading to being expelled a couple of times and kicked out of the Scholastics Honor Society (I learned later that a week before graduation my six teachers were polled to see if I should be allowed to graduate; I won 4 to 2). In particular, my frustrated math teacher (Hinshaw) predicted that I would end up working in the lettuce shed and playing chess in the park.

For all the years of living in farm towns, my dream was to live in LA (and I have been here ever since). In those days engineering at UCLA was just starting. Because of limited space, only about 40 students were allowed to come in as freshmen. The dean (Boelter) believed that engineering would change so rapidly that the traditionally trained engineer would be out of date in 10 years. Consequently, we had no specialties such has electrical, mechanical, chemical, etc. Everyone took the same circuit analysis (electrical, mechanical, and acoustic circuits) and the same field theory (Maxwell's equations and Navier−Stokes equation). We had a required lab every semester covering all areas of engineering. (The curriculum changed back to a standard one after Boelter left.) My only chemistry course was freshman chemistry, which I hated (memorizing organic names and colors for metal complexes). The only part I liked was the description of atomic structure. The sophomore engineering course exposed me to an atomistic view of materials science (Frankel), which I also liked. Since I liked atoms, I figured that I should become a nuclear engineer and wrote to the six colleges that then qualified for an AEC fellowship in nuclear engineering. MIT was clearly the best with two pages of courses (Caltech listed only two courses), and I decided then to attend MIT. The MIT catalog listed all of the courses that they expected applicants to have, and I planned my whole college curriculum around these courses. At that time, UCLA engineering was mostly in temporary buildings, but the students (Engineering Society of UC) operated a lounge with coffee (3¢), tea, and donuts. It had many large tables, and the entire faculty and students came to have coffee all through the day. Consequently, we had lots of casual contact with the professors. I was president of ESUC my senior year, giving me even more contact.

One of my professors was Paul Pietrokowsky, who ended up having the most influence upon my career. (Pietrokowsky had worked as a technician at JPL developing Ti alloys for Pol Duwez who then became a professor of materials science at Caltech; Pietrokowsky then got his Ph.D. in engineering science with Duwez in 1959). In my senior year Pietrokowsky was an acting Assistant Professor at UCLA who taught a special topics materials course. This course was amazing. We covered the Mathieu equation and band theory, donor and acceptor impurities in semiconductors, Chelikowsi growth of high-purity Si crystals, the 32 crystallographic point groups and stereodiagrams, the common crystal structures, X-ray diffraction extinction rules, the theory for transistor amplifiers, the Hall effect, and thermogalvanic properties. I particularly remember being given a powder diffraction pattern to interpret as a homework project. It was for Ti_3Au, which exhibits the A15 crystal structure characteristic of the (then) high-temperature superconductor metals. This was an unreasonable assignment, but with great luck, I got it right. In this course (spring 1960), Pietrokowsky told us that the future in electronics was to use metallurgical techniques to make integrated circuits that would have built into them the amplifiers, capacitors, inductors, and resistors of electronic devices. It was this course that excited my interest in materials. [Another student in the same course, Ron Lindh, was similarly stimulated. Ron also came to Caltech and worked with Pol Duwez, getting the first Caltech Ph.D. in materials science, founded a company, and is now an influential Caltech trustee).]

A month before coming to UCLA as a freshman, I met Amelia Yvonne Correy in El Centro (she worked for the County and applied for a loan from the Imperial County Credit Union, where I worked part time). Consequently, all my weekends at UCLA were filled visiting Yvonne in El Centro or Rosarito Beach (where her mother had a beach house). The result was that we totaled both of our automobiles (falling asleep), I got my only two B's in technical courses, and I spent all my savings. With my savings gone, I quit UCLA during my freshman year and worked for Douglas Aircraft Company as a tool designer (my drafting experience being the key to getting a good job; thanks, Mom). Here, I worked on tools for manufacturing the navy A3D fighter and the control trailers for the Thor missile system. Yvonne and I got married in October 1957, and I came back to UCLA motivated to study hard (for the first time) and excited about being an engineer (at Douglas I was using handbooks to figure out how to calculate moments in beams and to select the aluminum alloy appropriate for each application). Our son (Bill IV) was born during my junior year. Yvonne was fired from her job as a secretary for getting pregnant, but we had $40/week from unemployment. (I remember unpleasantly living on $12/week for food). With a son, I was planning to quit college and go to work again. One of my friends (Irwin Maltz) mentioned to his advisor (Bussel, who taught circuit analysis, in whose class I had been top student) that I was going to quit. Bussel then hired me as a TA to grade homework and exams. I was paid by the hour but was very careful, taking many hours to do the grading, with the result that we were able to finish my junior year. By then, in response to Sputnik, the U.S. instituted National Defense Education Act loans for students in science and technology, and we were able to borrow enough to supplement the meager UCLA scholarships of those days and the TA-ship to finish my senior year.

I had applied for the AEC nuclear engineering fellowship and also for an NSF graduate fellowship. Then I learned that I had to choose between them. The pay was the same (∼$2400/year for a married student with child), but Pietrokowsky advised me to take the NSF, good advice since I later decided to do materials science research rather than nuclear engineering. I applied only to MIT nuclear engineering and was accepted. However, by the end of my senior year, I calculated that I could not support a wife and child on the NSF fellowship. There was the possibility of NDEA loans, but at UCLA there was far too little loan money for the students in need and I assumed the same would be true for MIT. Consequently I got a job as a Research Engineer for Atomics International (part of North America Aviation, now Rockwell International), where I designed the heat-transfer part of the SNAP 10 nuclear-powered satellites. I decided that I would get a Masters degree going to UCLA part-time while working full time and saving money to go full time for my Ph.D. at MIT. I needed three recommendations for the UCLA Masters program, one of whom was to be Pietrokowsky. Although Pietrokowsky was by far the best instructor I ever had, UCLA had let him go after 1 year. His message that the materials scientists were wasting their time unless they went into semiconductors was not appreciated. I went to Paul's home where he explained that I would be crazy to give up the NSF fellowship. In addition, he said that Caltech was the place for me. I responded that Caltech had almost no courses in nuclear engineering, and he explained that in graduate school the important thing was research not course-taking. He also told me that Caltech had lots of loan funds and that I could borrow whatever was needed. Next week (mid-August) I got an application form from Caltech (Paul had arranged for it to be sent), and a couple of weeks later he bugged me to submit it, which I did around the end of August. In about a week I got an acceptance and took off a day to visit Caltech. I found out that I could borrow whatever the NSF did not cover and indeed that I could get the full amount of NDEA loans. I also talked to the people in Engineering Science (Caltech did not start a materials science program for another year or two) and decided to get a Ph.D. with Pol Duwez.

Paul Pietrokowsky then gave me a list of books (Pauling's *Nature of the Chemical Bond*, Griffith's *Transition Metal Ions*, Ziman's *Electrons and Phonons*, Wilson's *Theory of Metals*, Kittel's *Solid State Physics*, Wells' *Structural Inorganic Chemistry*, Smith's *Semiconductor Physics*, Nye's *Symmetry and Tensors*, the Mott and Jones book, Seitz' *Modern Theory of Solids*, and a book by Hume-Rothery) that I should study while taking my five courses per term. This was the perfect curriculum, which formed the basis for my future interests. Engineering science required that all students get a solid grounding in classical physics, quantum mechanics, and advanced mathematics, and I also took the materials science courses and many other courses around Caltech. Particularly important was a year-long graduate course on crystallography (my only course in chemistry after the freshman year) by Jules Sturdivant, in which I learned space groups (classic papers by Seitz) and gained his insights into crystal structures. In addition, Rudolf Mössbauer (who arrived at Caltech as a postdoc the month I arrived as a graduate student but was rapidly promoted to full professor his second year after winning the Nobel prize) taught a five-term course on solid-state physics that filled many holes in my background. Also, Paco Lagerstrom taught a year-long advanced group theory course covering Lie groups, including SU(n) that was important to me.

The second electron microprobe built in the world was built in Duwez's lab by Dave Wittry in 1959, but it had been disassembled and moved to a new building. My first job was to get this completely home-grown device working again. This was accomplished, but it never really worked well, and a commercial scanning electron microprobe (SEM) became available in another year or two. During my first year, I realized that even with the NDEA loans I could not support my family on the NSF fellowship (our daughter Suzy was born at the end of my first year). By this time, Pietrokowsky had been hired by Autonetics (a North American aviation company) to form a team to implement his ideas about using metallurgical techniques to develop integrated circuits. I was hired as a consultant to help his team during the summer months each year (during which time I made 135% of my 9-month NSF stipend). At Autonetics I designed and built (with the aid of an excellent shop) a device for measuring the Hall effect and conductivity of high-resistivity Si crystals at liquid He temperatures). This process was extremely slow, since there were no experts from whom to learn experimental techniques. However, during these three summers, I learned a great deal more about materials science and electronic materials.

At Caltech Duwez allowed me to follow my own research interests (his group at the time was developing the rapid cooling techniques that led to the group's discovery of amorphous Ge and Si, of simple cubic metal alloys, of amorphous metals, and of many metastable structures). I was struggling to use the many concepts about the theory of metals I had learned to explain the enormous variety of structures and properties of metallic alloys. At the time, I was an expert on all of the crystal structures but found that most explanations that seemed to work on the examples cited in the papers would fail on other systems I knew about. This gradually led to the idea that I would have to better understand the bonding in metal alloys. At the time, I felt that all computer calculations were so extremely approximate that they were useless (I no longer feel this way). I felt that the only reliable understanding had to come from group theory and selection rules. I felt that this might not be possible for gross crystal structure but thought that it might be possible to explain the structures of antiferromagnets. I knew that among the rutile structures there were several that were antiferromagnetic, exhibiting several different patterns, and that others (e.g., VO_2) exhibited a variety of distorted crystal structures. I found that I could explain all of these structures using the Heisenberg exchange Hamiltonian with a particular variation in the exchange operator with distance. I then wanted to calculate these exchange operators but soon learned that this would be very difficult to do from first principles. Indeed, it was not clear to me that the theory was well founded in quantum mechanics. I knew about some oxyfluorides that had three metals strongly interacting but weakly coupled to their neighbors and figured I would try to predict the spin coupling. I struggled with developing ways to deal with wave functions that led to proper spin eigenfunctions while satisfying the Pauli principle. Since I was an expert on group theory, including the symmetric group and SU(2), I was able to figure out a way to develop a group operator that would do this. However, I learned that this would give general rules on the order of the spin states only for one-dimensional systems.

I then realized that by using this group operator with a product of spin−orbitals, I could develop a way to determine the optimum shape of the orbitals (the GI method), which I hoped would give insight into the nature of the bonding. I struggled to derive the equations. (I had heard of Hartree−Fock theory but was not familiar with the details.) I was able to show that it was permissible for the optimum H_2 and CH_4 orbitals to be partially localized on different atoms but still satisfy the Pauli, spin, and spatial symmetries. At this point I wanted to actually solve the equations; however, I had not learned to program a computer and my four years of fellowship support was up (during my fourth summer, Duwez supported me, so I did not need to consult).

With 6 weeks before the end of the NSF, I started writing the thesis covering all 4 years. In 3 weeks I had the first draft, but Duwez felt that no one in engineering science would understand it [actually, Milton Plesset, a specialist in nuclear engineering, was on my committee, but he never read far enough to see my discussion of the Moller−Plesset theorem (the basis of MP*n* methods) and its relation to the GI method]. Consequently, a professor from physics and two from chemistry (Sunney Chan and Russ Pitzer) were added to my committee. I had not met them before giving them a thesis to read. The Ph.D. exam went well, but Chan rightly complained about my writing, which was terrible. I struggled over 2 weeks to improve the writing well enough to satisfy Chan. During this time he asked me what my plans were. With my NSF over, I knew that Duwez would support me for a time while I wrote up the thesis into papers. I assumed that I would then get a job as an experimentalist in the aerospace or electronics industry. But with a wife and two children to support, I had not yet applied for a job (even then putting things off to the last moment)! By this point, I really wanted to learn how to program a computer to apply my theory to real molecules, but I did not expect to find such a job (I still did not realize that one could do theory as a full time occupation). Chan asked if I would like to join the chemistry staff (in a nontenure track position as a Noyes Fellow), and I jumped at the idea, starting November 1, 1964.

The first month I learned to program (in Fortran II by borrowing some code from Pitzer and going through it line by line) and solved the H_2 problem as a function of distance. Indeed, the optimum orbitals did localize and did dissociate properly! The second month I did the Li problem, where there had been strong interest in predicting the spin density at the nucleus. HF led to poor results, while spin-unrestricted HF (UHF) was much improved. There had been speculation that optimizing the orbitals after spin projection would be even better. The GI method did exactly this, and it did work. The next 9 months were spent developing a general computer program and writing the first three papers. Again, Chan played a special role in helping me learn how to write effectively, while Pitzer helped by letting me use his Cambridge Polyatomic Integrals code. After some problems with referees, these papers eventually came out. Meanwhile I got offers of tenure track positions at Caltech, Harvard, and MIT. Although at that time Harvard was clearly the most exciting place to do theory, Chan talked me into staying at Caltech (no doubt the right decision).

With the help of a stream of amazingly gifted graduate students (and postdocs and undergraduates), we were able to develop the new methods and apply them to an increasing diverse array of problems. In the process, I gradually learned chemistry, which I know now to be my true love (along with Yvonne). It is certainly a great country that permits a poor farm boy to find a way to end up having such fun figuring out how materials work.

I dedicate this volume to the teacher (Paul Pietrokowsky) who most influenced my career, to the colleague (Sunney Chan) who most shaped my early evolution into a chemist, to my loving wife (Yvonne) and our four children (Bill, Suzy, Cece, and Lisa) who have tolerated my dedication and love of science, and to my research group (see List of Colleagues of William A. Goddard III) who have made the enormous progress for which I get too much credit. Listed are the graduate students, postdoctoral fellows, undergraduates, and colleagues that have actually written published papers with me. Section 1 lists those that received advanced degrees from Caltech while working with me. The ones whose graduate research was primarily with another faculty member have an asterisk next to the faculty member's name. Section 2 includes others that were postdoctoral fellows and undergraduates of visitors with me, while section 3 includes colleagues at Caltech and elsewhere who have collaborated with me on published papers. The time periods quoted are roughly those that led to published papers.

I would like to thank those (particularly Rick Muller) who organized the surprise 60th birthday meeting at Caltech (which I did not learn about until about a week earlier) and those (particularly Emily Carter, Thom Dunning, and Ellen Stechel) that helped put together this issue. In addition, I would like to thank those that traveled far and near to join me in the celebration. This included Guanhua Chen (Hong Kong); Terumasa Yamasaki (Japan); Wilson Ho, Dick Messmer, Rich Friesner, and Bea Botch (New York); Fritz Schaefer (Georgia); Mo Li (Maryland); Don Tomalia (Michigan); Larry Harding (Illinois); Larry Yaffe, Thom Dunning, and Ray Bair (Washington State); Peter Armentrout (Utah); Barney Ellison and Sally Sullivan (Boulder); Tony Redondo, Art Voter and Jeff Hay (Los Alamos, NM); Steve Walch and Guanghua Gao (Northern California); Mike Bower, Seung Koo Shin, and Bill Palke (Santa Barbara).

William A. Goddard III