12724 J. Phys. Chem. A 2008, 112, 12724–12736

Autobiography of Sason Shaik

This is a story of science and friendship, which starting in 1979 is based on a diary I have been keeping. If I had to summarize this story in a single sentence I would have chosen to say: “I have been a fortunate guy to forge many friendships and to be excited about my science”. To start where I started and to reach this point in life when many friends, students and colleagues contribute papers to honor me makes me feel very fortunate. I was born in Iraq to a Jewish family. My father was a jeweler, sort of an artist, in a tradition of his forefathers. My mother was a very young woman (of 18) when she had me, and soon enough she gave birth to my brother Mordecai. These were bad days for the Jews in Iraq because of the wave of nationalism that swept the country. The establishment of the state of Israel only worsened the situation; it was risky to remain in Iraq. Most of the Jews of the country had to leave, and their properties were confiscated. My parents were among these refugees. So from a fairly rich family living in a bustling metropolitan city like Baghdad, they found themselves without a penny, and with two little sons living in a transit camp in a tent in the middle of a desert.

I was too little to remember anything, and my first dim memories are from this transit camp (now a thriving city of the high middle class near Tel Aviv). In my mind there is a picture of a tent and a lot of sand around, though it may be just the picture that I painted for myself from the stories of my parents. Somehow my parents managed to overcome the hardships, leave the transit camp and move to a southern suburb of Tel Aviv, so-called “residence of the hope”. This was a flat-low neighborhood, which in every serious winter would be flooded (still is). My second strong memory is me and my family standing on the roof of the building where we lived, in a ground floor apartment; below there were men in boats and my father carried each one of us and threw one-by-one to the boatmen. There was no place for him and he had to swim his way and find us in one of the schools where all the escapees of the flood were temporarily lodged. In the “residence of the hope” I started going to school. Then, when I was six and a half-years old, my parents moved to Ramat-Gan (“Garden-Hill”), the city where many of the Iraqi immigrants flocked. My father died quite soon after the move and my mother carried on with the duty of maintaining the family all by herself. There in Ramat-Gan I continued my schooling, discovered books, which became my good friends, and then I discovered chemistry.... In retrospect, I was fortunate already then, because education was a high priority in the young state of Israel, and there was vision, and there was encouragement of good pupils, what we call today in the typically worn out term “excellence”. I was fortunate also because I grew up in a young dynamic and equal-opportunity society, where what mattered was my success in school. So, I owe a debt of gratitude to my country of immigration.

My elementary school in Ramat-Gan was in an orange orchard, and it was fittingly called “Pardes”, namely “Orchard”. It was enchanting each morning and noon to walk through the trees and imagine things. Indeed, I was quite a usual kid—I liked wrestling, soccer, organizing “wars” against other neighborhood groups, and daydreaming in the orchard. My most beloved teacher, Herschman, was a great storyteller, and he used to tell us every Friday a little bit of the voyages of Odysseus. He was so gifted that still to this day I can call upon the images of the Odyssey and see them vividly as in a movie. My love for books and for literary self-expression developed then, and Herschman encouraged both loves. But in my early teens (12−15) I began to like also chemistry and to fiddle with chemicals. In those days you could go to the pharmacy nearby (or send your mother) and purchase a few chemicals, like sulfur, potassium permanganate, potassium nitrate, HCl, etc. There was a store for photographic equipment where you could buy some more chemicals, and there was the laboratory in school.... I had red phosphorus, potassium and sodium, zinc, sulfuric acid, nitric acid, hydrochloric acid, yellow sulfur, mercury, carbon pills, an oxide of mercury, iodine, sodium thiosulphate, hydroquinone, $K_4[Fe(CN)_6]$, $K_4[Fe(CN)_6]$, the Bertholet salt, copper sulfate, NaOH, KOH, and so on. When I started high school, I already had some knowledge of chemistry. I got a hold of a book that had recipes for making “gentle” explosives that scared the old neighbor who used to chase our soccer ball, smelly gases (H_2S) that irritated the teacher, igniting hydrogen that was liked by my little brother, and many others. I tried most of them, and improvised others by mixing chemicals and grinding them or heating them. One day I “discovered” the gas chlorine; I mixed potassium permanganate with HCl, and a vigorous effervescence occurred. I stuck my nose in and took a deep breath; I almost chocked. I still tell my students, now in the course History of Chemistry, that a chemist is one who likes to mix materials, smell them and taste them. I liked color changes, of $CuSO_4$ when heated and then recooled, of PbI_4 that gave “golden leaves”, of the crimson red of the permanganate solution and how it changed quickly to brown and then transparent when I added some chemicals to it (e.g., sulfites or thiosulfite). This is “the magic of chemistry”, as I now tell my students in History of Chemistry: “*a substance disappears and a new one appears*”. When I turned 15, I had to choose either natural sciences or humanities; the latter meant “no more chemistry”. I was torn between my love of humanities and literature and my love for chemistry. I ended up choosing natural sciences, I suspect because I loved chemistry, which was so much fun. In the years to come there were days I regretted my choice, but there were other days where I was very happy, especially when we were in the chemistry and physics laboratories, playing with chemicals, electricity, magnets, fluorescence and so on.

It was then when I bought my first camera, and started developing my own pictures. Photography was ideal because I could combine my joy of chemistry with my new love. I used to mix chemicals, change relative weights of ingredients and watch how this affected the picture. It was magic, “the magic of chemistry” again: images appeared, got fixed, and could be made to disappear and be dyed. I spent hours in the darkroom. It was a tiny little bathroom with a bathtub that almost filled the room, and I used to sit in the tub, on a little bathing stool (habitually found then in Iraqi families), and all the equipment and chemicals would be spread around. I used to sweat profusely inside the little room, and many of the times my younger brother used to join me, and we would both sweat and marvel at the wonders of the little silver grains that slowly joined and made up the pictures. This double flirt with chemistry and photography continued through my army service.

In my country army service is compulsory and so, in 1965 I enlisted and became a soldier in the Israel Defense Force (IDF),

10.1021/jp806625w CCC: $40.75

in which I served for three years, and finished the service a year after the Six Days War. When I completed the service, it was time to go to the university. Again I was torn between humanities and natural sciences, and again I let my special love for chemistry decide for me. I joined the chemistry program in Bar Ilan University. This was a heavy load of studies, many laboratory courses, chemistry, math, physics, etc., and many inspiring teachers. Suddenly, there was something more exciting than the laboratory (which at the beginning was easy for me anyway): I was taught about these creatures called orbitals and was immediately enchanted; they attracted my imagination. I practiced a lot to draw these orbitals, and one day I drew on the blackboard my general chemistry teacher, the late Yaakov Goldschmidt, waiving at us a d_z2 orbital. Suddenly, he entered the class and I froze; "he will probably ban me from his class" I thought. To my surprise he smiled, wiped out his drawing and left the orbital, and continued to teach from there. I also discovered mechanistic chemistry and structure determination by spectroscopy. It was so exciting; I was thrilled to push arrows and to figure out how to prove a mechanism, or to decipher a spectrum. Then came quantum chemistry, which was taught by Harold Basch; there were the particle-wave duality and other oddities, which intrigued me and made me feel I am learning something really important. One of my most remembered teachers was Milon Sprecher, a rigorous teacher with a vast knowledge and a special gift for teaching. He taught us mechanistic organic chemistry, and his teachings are still engraved in my mind. He then taught us symmetry in chemistry—a beautiful course. Chemistry was beautiful and exciting! I was slowly being converted to become a theorist, but I did not know that at the time.

In 1972, I finished my B.Sc. studies and decided to continue my M.Sc. studies in experimental chemistry and joined Michael Albeck's group. He was doing polymer chemistry then and started doing tellurium chemistry, following findings of Zvi Rappoport (who is now my colleague) and his students of π-complex formation between olefins and tellurium tetrachloride. The topic of π-complexes sounded quite exciting to me, and I wanted to try it. Very quickly I found out that my skills in chemical synthesis, isolation, purification, etc., were not outstanding. I was too impatient and these experiments were hard and tedious. Tellurium tetrachloride is a powerful oxidant, and all my spatulas were turning black as soon as they got near $TeCl_4$. It was also very reactive and converted every organic compound, which I felt could form a π-complex, into a black paste. Soon, all my spatulas were destroyed; my flasks were filled either with the black paste, or with some white sticky emulsion due to hydrolysis of $TeCl_4$. I was desperate! I began using Teflon spatulas, working in glove boxes, drying all my glassware and keeping them in large desiccators. Nothing much helped, the black paste was still forming, and I could not isolate anything. One time I saw beautiful large orange crystals in the flask. I turned quickly to write in my notebook what was precisely done, so I could repeat the experiment when needed. When I looked again at the flask, the crystals had disappeared.... The magic of chemistry was playing tricks on me.

During my MSc studies I took a few courses. I had two courses in physical organic chemistry, one in mechanistic chemistry from Shmariahu Hoz. I found that I liked to think about mechanisms and to take courses in theory. One of the courses that left on me an everlasting impression was a course in molecular orbital theory given by Millon Sprecher. He taught us everything from Hückel theory, to Dewar PMO, to SCF theory and all the way to the Woodward−Hoffmann (WH) Rules. I was fascinated by these orbital theories. It was then that I began thinking about going to the U.S.A. to do my Ph.D. studies.

While I was still struggling with the black paste, the Yom Kippur war erupted in October 1973 and I was called to serve in a reserve unit. Toward the end of the war my unit was sent to a captured airfield within Egypt. We lived inside the airplane shelters and we spent there many hours just sitting whether there were bomb alerts or actual ones. When you hide you tend to be quiet and focused. In one of these long hiding events, I suddenly saw the light and understood the nature of the black paste I was getting when I mixed $TeCl_4$, for example, with anthracene. I could clearly envision the anthracene attacking the chlorine center of the $TeCl_3^+$ moiety giving chlorinated anthracene and $TeCl_2$ that disproportionated and deposited elemental Te. I understood this mechanism through an orbital model of $TeCl_4$, which I mentally constructed, and which suggested that the actual structure of $TeCl_4$ in solution was $TeCl_3^+Cl^-$. When I was released from the army, it took me exactly one month to isolate all the chlorination products of anthracene and other aromatics and olefins, and identify by mass spectrometry all the Te and $TeCl_n$ fragments. I was happy, my teacher Michael Albeck was proud of the MO model and we wrote together the paper. This was a happy ending, and I felt fortunate again.... After the publication of the paper I got a note from Roald Hoffmann (who published a paper on SCl_4 I think) that he saw my paper and liked it, and was sorry he did not spot it on time to cite it. By that time I already was in the University of Washington in Seattle as a Ph.D. student of Nick Epiotis.

My "fortunate" application of MO arguments to a real problem convinced me that my destiny is to be a theoretician. I wrote to Roald Hoffmann, Ralph Pearson, and Nick Epiotis. Nick was a newcomer in the literature, and I was drawn to him because he published in clusters of four papers, and the ideas were very attractive and creative; I was taken by these ideas. All the three suggested that I first apply to the university and be admitted to the graduate school, and so I did. Roald wrote a usual cautious letter and suggested not to put all my eggs in one basket. Being inexperienced, this felt like a rejection, I was sad, because I wanted very much to work with Roald. Nick's letter was typically ebullient, The University of Washington replied fast, and so did Northwestern. I consulted Harold Basch, and he thought that Nick was a rising star and that the weather in Seattle is much better than Northwestern. In the meantime I was awarded a Fulbright Fellowship that enabled me to travel to the U.S. Because I was anyway taken with Nick's ideas, I decided to go to the University of Washington. Seattle was pleasant, the campus was beautiful, and the autumn leaves and the cherry blossom were gorgeous. In addition, I received a host family from the University, and they let me live in their home for the first month and took care to acclimate me in the new environment. This family (Porte) has become my second family and is still so to date. Having a host family when you are far away from your own family makes life easier and makes it possible for me to dedicate my energy to studying and research. I was lucky again!

When I arrived, Nick was on his annual vacation in the Greek Islands. In the meantime, I was settled in the department and was waiting for school to start and for Nick to arrive. We finally met in his office. He looked at me and was amused. He told me that the group (then Ron Yates and Bill Cherry were his students, later Jim Larson joined) was going to write a book and he suggested I join in, because he wanted to know "*what the genius from Tel Aviv*" could really do. This is how I started my Ph.D., I read like a madman and collected experimental data on structures and relative stability of molecules, and ran small calculations. In the end, I had to figure out how all the data fitted into a model of orbital interaction: hyperconjugative interactions, nonbonded attractions, and so on and so forth, were some of the buzzwords in the group. The book was eventually written and published in 1977 as volume 70 of *Topics in Current Chemistry*. It is still a good book and the ideas there are still timely.

During the work on the book Nick used to stimulate us and he knew how to do that very well, and I was very stimulated all the time; it felt like living on the foothills of a volcano. I still recall him telling us how he viewed patterns and existing models of explanation. He used to raise his voice and say: "*I toss the data in the air and it falls on my desk in a different order*"! I learnt this lesson very well, and I began to question everything I have known and learnt in chemistry. I used to read the literature with hunger to mine new and interesting data, so I could find new patterns. In the summer of the first year, when Nick went on his vacation to the Greek Islands, I sat in the Porte's house and wrote 10 papers. When he came back, I handed them to him: some of them survived and eventually became published papers. Then he told me, read my review in *Angewandte Chemie* and write a paper about organic photochemistry. The *Angewandte Chemie* paper by Nick dealt with looking at reactivity using fragment-based electronic configurations. I read the paper, took many notes, learnt the basic rules and wrote a paper. Nick took it, came back after a week and said: "*Good scholarship Sason*", and I never saw it again; it was never published, and in retrospect it should not have. Nick's unusual way of introducing starting Ph.D. students into research paid off, because I became independent very early during my Ph.D. and had a clear vision what my way in science was. I was fortunate again....

I attended many interesting courses at the University of Washington. I took physical organic chemistry from Fred Schubert and Isaiah Pocker, theoretical organic chemistry from Wes Borden and Nick Epiotis, Quantum Chemistry from Erny Davidson and Martin Gouterman, and so on. In Gouterman's course I learnt about spin−orbit coupling, and the constitution of the corresponding operator (as *L.S.*). One day, as I was walking on the beautiful campus, on my way to swim, I suddenly had a neat thought how the operator can lead to stereochemical consequences in organic photoreactions. I used the configurational approach developed by Nick and derived stereochemical rules for spin inversion. These rules showed that in 2 + 2 cycloadditions (e.g., of cyclohexenone and an olefin), one should get distorted *trans*-fused four-member rings, and how it preferred the photo Diels−Alder reaction; whereas in singlet state photochemistry both products where forbidden by the Woodward−Hoffmann rules. I was very excited; this was my first completely independent idea, and I could recognize that the idea was good and novel. Nick thought so, and so did Martin Gouterman with whom I consulted. Later I learnt that Lionel Salem published two beautiful papers on spin inversion in organic diradicals. I was pretty sad to find that I was not the first one to think about spin inversion and stereochemistry. But Nick assured me that my treatment was more elaborate and far reaching than the treatment of diradicals. I got strong encouragement also from Schubert and Gouterman. I sat down to write the paper. Nick decided I should get the asterisk. So here was my first paper where I also appeared as the "senior" author; this was a great gesture. Ever since that event, I used the same gesture toward students and co-workers whom I felt did some worthy and independent work.

During my Ph.D. time, Roald Hoffmann visited the University of Washington and gave the H. Dauben lecture series. As Hoffmann likes to do, he invited all the students for beer in the local pub. It was a great opportunity for all of us to sit in the company of this famous chemist, who by everybody's view was a future Nobel Laureate. In the relaxed atmosphere of the pub, I gathered enough courage to ask him what he thought would be the future trend in quantum chemistry. He answered in his typical thoughtful manner and said many things I did not understand then. But one thing struck me the most: He was predicting that VB theory would make a comeback! Considering the consensus then on VB theory, what Hoffmann was saying sounded at best strange, and I thought to myself "*Does not he know that VB theory is passé and is anyway a wrong theory*?" Not much time later, toward the end of my Ph.D., I suddenly found myself discovering VB theory and falling in love. The exercise I did with the configuration approach of Nick had started me thinking how can I "prove" that these configurations are parts of the MO (or MO-CI) wave function. I have begun to devise a method to expand the MO wave function to such configurations, and I could see that some of the terms I was getting included atomic orbitals and looked like VB structures. I started reading about VB theory and the little I could find in books convinced me to continue in this manner because the theory provided a clear picture of the bond. But there was no time to pursue this interest, I needed to write my Ph.D. thesis, and relax from intense days at the foothills of the volcano. I left the MO-VB matter unresolved and made for myself some notes in my notebook.

This was the time to search for a postdoc position, and I was determined to go to Roald Hoffmann. I wrote to him again, and his letter again advised me not to "*put all the eggs in one basket*". A rejection again? I was sad! So, Nick called Roald and talked to him about me. The next thing I heard from Roald was an offer to join his group as a postdoc. I joined the group in the summer of 1978. When I arrived in Ithaca, Roald was away in England, and I took some time to settle down. Roald's secretary found for me a room in an apartment (in "Lucenti Homes"), which I shared with three Ph.D. students; two of them, Cynthia Burrows and Barbara Baird are today Professors in Utah and in Cornell. Just nearby was living Evgeney Schusterovich who left Russia and was a visitor in Roald's group. Ithaca was a small place, with a population that was equal or smaller than the number of students who attended Cornell, such that wherever you lived you would find many students. And, the winter was cold, bitter cold! I have never been before in a cold country (other than going to ski when I was in Seattle), and there was much to get used to, including to learn how to drive on snow. The first time I tried, I found myself without any ability to control what the car was doing. Living with students and being in a university environment all the time helped, and I learnt how to manage and how to open the frozen lock of my car in the morning.

I spent one year in the group. This was one of the best years of my life, in terms of intellectual stimulation and lasting friendships; all of which I cherish to this day. The members of the group were Robert D. Bach, Eluvantigal D. Jemmis, Al Pinhas, Dave Hoffmann, Charles Wilker, Kevin Haraki, Tim Hughbancks, Brigitte Schilling, Armel Stockis, Christian Minot, Kaz Tatsumi, and Evgeney Schusterovich. This was a very stimulating group of different nationalities and a variety of backgrounds; some were experimentalists who came to learn the trade from the Rabbi, and others were theoreticians who wanted to learn how to think about the calculations and not only to generate numbers. Brigitte Schilling, from Denmark, was responsible for training me in doing calculations with the local Extended Hückel program (maintained by Kevin Haraki). When Roald arrived, I was already well versed in the calculations. Roald used to hold systematically at least one group meeting every week; this will last any number of hours starting lunchtime. During these meetings, sometimes we gave seminars, but most of the meetings Roald would bring transparencies with problems he collected in the daily or weekly reading. He would then show the transparency and would analyze the problem on the blackboard using orbital language. He was teaching us every instance he could. Sometimes he would bring a book on science but not a scientific book, and he would recommend it, or would simply tell us about it. Roald was interested also in art and poetry, and when he learnt that I was writing poetry, he exchanged poems with me. It was a great feeling to be able to feel that doing science need not be only a narrow focusing, but that it benefits from all sorts of creative activities. The group was friendly and dynamic and we used to have many arguments: I used to discuss my scientific ideas a lot with Jemmis, Bob Bach, Al Pinhas, and Dave Hoffman. This open-minded atmosphere made you feel like being in the school of Aristotle, and it evoked whatever creativity you had in you. I used to write many sayings and aphorisms, and paste them on the doors of the huge aluminum cabinet where we kept all the outputs. Roald would look at them bemused; he let them hang around long after I left. Roald's group was frequented by many prominent chemists: To mention but a few, I had a chance to meet Harry Gray, Dick Schrock, Jean Marie Lehn, Lorenz Cederbaum, Thomas Albright, Mike Whangbo, and so on. Another stimulating personality was Evgeny, a terrific theoretician who worked only analytically. In Russia he calculated ferrocene at the CNDO approximation and solved all the necessary integrals and the diagonalizations all with "paper and pencil". So, he knew a lot of tricks, which he would tell me about enthusiastically during our lunch walks in the campus.

The focus of the scientific activity in the group was organometallic and inorganic chemistry. I knew little organometallic chemistry and did not seem to care about it at the beginning. I was hung up on my spin inversion theory and my MO-VB mapping. I wrote three papers on spin inversion, one of them called "*Spin Inversion and Orbital Symmetry Conspiracy*", a nice catchy name I found for describing photoreactions where the stereochemical requirements of both the Woodward−Hoffmann Rules as well as my own Spin Inversion Rules could be satisfied by the same reaction coordinate. I gave a talk in the group and Roald seemed to have liked what he heard. I was then invited to give this talk in Mel Goldstein's group. I felt very honored to get this invitation from a prominent organic chemist.

Because I felt guilty I was not doing anything with Roald, I thought to put his name on my papers, and showed him the first drafts. He called me to say that it was not necessary and said: "*I am happy Sason that you are independent. I will tell you when I want you to do something*". A few weeks later he invited me to his office and asked me to look at the Vahrenkamp compounds, which were bridged bimetallic complexes with a variable M−M distance that seemed to depend on the d-orbital count of the metal. Soon after that time, I was well into the various organometallic projects with Roald. I read his papers on the "*isolobal analogy*" and the "*through space and through bond*" model and heard him talking about the analogy in the group. One thing that attracted me was the orbital acrobatics he was doing to derive these models using alternately delocalized and localized MOs. It was clear that there is great advantage in moving between the two worlds, and in using insights of both representations. I fiddled with these transformations for the Vahrenkamp compounds and created localized MOs for the M_2X_2 bridge unit.

Crossing the mirror between the worlds was a lot fun. This has strengthened my feeling that I should continue with MO → VB projection to understand better chemical reactivity. Even though I was busy at that time with my organometallic and inorganic projects, I still found some time, and developed the machinery to project the wave function systematically. I realized that to comprehend reactivity I should fuse the insights of the two theories in a manner that will allow me to understand chemical reactivity in a unified scheme. I got some exciting trends, everything I set for myself seemed to be in my hands: a general mechanism of barrier formation, a general understanding of the origins of reaction intermediates, and an easy way to predict the preferred stereoselectivity of reactions, even for odd electron reactions, which is not possible to achieve by MO arguments. I finally had a VB model of reactivity that created a bridge to MO and MO-CI wave functions. I did not have the time to write the paper, because according to the rules of the Fulbright Foundation, I had to leave the U.S. and spend at least two years in Israel before I could go back to the States. Luckily, I got an offer from Ben Gurion University in Beer Sheva, so I had a place to return to. I was lucky again.

Coming to Israel after five years in the States was somewhat of a culture shock; this was not the country I remembered, nor was I the same person who left it. Interestingly, Beer Sheva was a sister city of Seattle, so at least there was a familiar name. I got a university apartment at the edge of the city, and this edge was on the border of the desert. Every morning I would see from my window the sandy horizon and the young Bedouin shepherdess with her herd of goats. There is a lot of charm in the desert but it takes getting used to. Ben Gurion University was established in the Negev as part of Ben Gurion's vision to settle the desert. However, soon enough the budgets for building and development were cut off, and the young University was severely held back. But the department in Beer-Sheva was young and the atmosphere was dynamic and free....

I did not have an office for a few years and so I occupied the offices of my colleagues who were on sabbatical; I think I sat in Addy Pross' office who was then in Australia. Other than teaching (first year general chemistry to biology and geology students) I did not have any other duties, and I could sit in my office or stay at home and write the paper on spin inversion in Diels−Alder reactions, and the first paper on a VB model of reactivity. I completed the Diels−Alder paper first, submitted it and it got accepted quite fast. Then I completed the VB paper, and after having written it, there came out a unified general picture of reactivity that was applicable to any reaction type and was derived from quantum mechanics with no ad-hoc assumptions. I always viewed this work through the metaphor "LEGO"—the children's game in which you build the "whole" from building blocks. I thus found the building blocks of energy profiles, transition states and reaction intermediates, and was going to show how to reconstruct these "chemical reactivity objects" and conceptualize them using these VB building blocks. I was so pleased with the outcome that I gave the paper the title, "*What happens to Molecules as They React*?...", that reflected my excitement about the work. I was sure it would excite everybody. After a long struggle with the referees, the paper was finally accepted and appeared in 1981, more than one year after submission. In those days, we did not rely on citation indices, but on reprint requests, the little cards that said, "*please send me your paper*...". I got more than 300 cards, and this was a great feeling. Later when I would struggle to publish my VB papers, I realized that much of the interest could have been caused by the catchy title rather than by the genuine interest in the work. Now looking at the citation statistics of this paper, my conclusion is that the truth is somewhere in the middle.

In the meantime, Addy Pross returned from his sabbatical and came to his office where I was sitting, I was on the way out to move to another office. We started talking and he asked me what I was doing. I described to him my work on spin inversion, which he liked. And then I described the VB model. He asked me "*what can you do with it*"? Finally, I had a captive audience, so I told Addy what I thought were the many potential uses of the diagram for discussing relative reactivity, stereochemistry, and reaction mechanisms. I recall his eyes lit, he was a physical organic chemist and the model was specifically addressing the agenda of his field. I gave him the submitted draft of the first paper, and after a few days he came back to me and suggested that we collaborate on the S_N2 reactivity of benzyl derivatives. I immediately agreed and this turned out to be an intense and fortunate collaboration. Addy was a fast writer and very familiar with the field. The paper passed quite easily through the *JACS* referees, and ended up being published in 1981 back to back with the theoretical paper on "*What happens to Molecules as They React*?..."

In 1980, immediately after having developed the VB model, I was seeking for ways to apply it in a semiquantitative way, and to see how well it could interact with the experimental data. John Brauman was publishing his wonderful work on gas phase S_N2 reactivity, and derived barriers for identity reactions, where the nucleophile and the leaving group were identical. This was an ideal case for application of the VB diagrams that I derived, and I started thinking about the application. According to the VB model, the barrier for the reaction was given as $\Delta E^{\ddagger} = f\mathrm{G} - \mathrm{B}$, where f was the fraction of the promotion gap G that entered under the crossing point in the VB diagram, and B was the resonance energy mixing of the two VB states at the crossing point. The equation was simple and pretty but it required articulation. I figured out the chemical factors that controlled the various quantities for the identity S_N2 reaction, and submitted a communication to *JACS*. It was rejected after a long struggle and would eventually be published in 1982 in the French Journal, *Nouveau Journal de Chimie (NJC)*.

I was continuously thinking about a way to make the scheme quantitative. In June 1980, I married Sara, and because I had a DAAD fellowship we went together to Heidelberg to spend two months with the group of Lorenz (Lenz) Cederbaum, whom I met in Cornell. How did I get away with a honeymoon in the chemistry department in Heidelberg is one story I will leave for my grandchildren. In addition to Lenz, the more senior members of the group were then Köppel, Jochen Schirmer and Wolfgang Domcke. All of them have remained close friends to this day, and in December 2007, when I visited Heidelberg again as the Christams Lecturer, Sara and I met the group, and we needed no time to bridge the 27 years that passed. The other part of the story was the scientific work I did I Heidelberg. The Heidelberg group originated in physics, and worked among other things on vibronic coupling in ionization processes in molecules (especially Lenz, Köppel and Domcke). The vibronic coupling mechanism often involves state crossings and avoided crossings, and it looked like the right stuff for me to learn. Although I had a good intuitive understanding of what they were doing, there was a language gap; many terms have had to be translated from Physics to Chemistry. Often times I was at a loss. Luckily, there was Andreas, a Ph.D. student who came from chemistry. I used to sit with Andreas every day for about half an hour and we would go through the book of Vetter and Valecka and translate the stuff into a more chemical language. After a short while, I felt at ease with the language and I decided to initiate a review in *Angewandte Chemie* on the problem of symmetry breaking and non Born−Oppenheimer effects in cation radicals, where I showed the substituent effects on the vibronic coupling, and the other group members contributed their parts. Physicists tend to describe complex phenomena in terms of simple analytical models with effective parameters; I especially needed f values and I could pick up enough to articulate my own barrier equation, $\Delta E^{\ddagger} = f\mathrm{G} - \mathrm{B}$, and use it to calculate barriers for identity and nonidentity S_N2 reactions. When I came back from Heidelberg, I wrote with Addy a full paper on S_N2 reactivity of CH_3X derivatives, where the barrier equation was applied quantitatively; we managed to show that it captured the physical essence of the S_N2 reaction in the gas phase. I was very proud of the paper because it interacted so well with the experimental data and could make predictions so easily and lucidly.

By that time I was wary of *JACS* because quite a few of the papers I had written during that time were getting rejected or met with serious difficulties. I was desperate; the communication on the identity reactions was rejected, and I was concerned for the fate of the full paper. I hedged, and decided not to submit the paper until I could speak to Roald, whom I was going to visit in the summer of 1981. Coming to Cornell was like coming home. I showed Roald the referee reports I was getting and asked his advice. He went to his small backroom, and came out with a bundle of referee reports on his own papers, and said: "*sit and read these*". I read, and could see his point: my share with the referees was not different than others'. Then he gave me advice about the two S_N2 papers, and in the end the communication was published in *NJC* and the full paper in *JACS*.

The years 1982−1984 were very intense: I collaborated with Addy on applications of the model to as many reaction mechanisms as we could. Joe Bunnett, then the editor of *Accounts of Chemical Research*, invited us to write a short review. I was working on the theory of organic conductors made from donors and acceptors and their isomeric charge transfer complexes (published in 1982 in *JACS*). I derived rules for designing organic conductors with controlled stoichiometry and degree of charge transfer and convinced some of my colleagues J. Bernstein, J. Y. Becker, and S. Bittner, to team and tackle the topic from different angles (crystallography, electrochemistry, and synthesis). So, we formed the "*Organic Metals Group*" at Ben Gurion University, and in the current terminology we were doing *nanochemistry*—only in those days it was not called so. The group existed from 1983 till 1991, and although we did not manage to make a real breakthrough, it was fun while it lasted. Simultaneously, I kept developing the VB model: In 1983, I published the paper on α- and β-carbon substituent effect in S_N2 where I utilized the model to make some counterintuitive predictions on the effect of strong electron withdrawing substituents, which years later were verified by experiments in the gas phase. In the same year, 1983, I managed to incorporate solvent effects into the VB diagram, so I could estimate S_N2 barriers in many solvents, the paper was published in 1984 in *JACS*. I finally had in my hands a model that was making qualitative as well as semiquantitative predictions.

Still in 1983, my friend and former classmate, Ronny Bar, from the B.Sc. days in Bar Ilan, called me and asked if she could do again (she had done so in 1980 and then stopped) some research with me. Ronny was a rich lady, who wanted to do research for intellectual stimulation. She was a superb student, and I was fortunate that she wanted to do research. We did two projects together, the second is the more interesting.... Already in 1982, I had a crazy idea that in fact all the π-electronic components of delocalized systems like benzene and allylic species, were in fact transition states trapped by their σ-frames. In those days, I used to sit every Friday in Café Fredo in Beer-Sheva with my friend Oded Israeli (a great painter), and just watch the world go by. In these rare moments many ideas tend to surface; Oded would paint his, and I would write papers on mine. The idea on the π-electrons of benzene surfaced in one of these Fridays, as suddenly it struck me that if I apply the VB model only to the π-electrons, the quantitative prediction would be that the delocalized π-electronic system was a transition with a sizable barrier, and hence in the real D_{6h} molecule it must be held forcefully by the σ-frame. Ronny Bar did the calculations with Extended Hückel and we could show that the π-electronic components of allylic species were transition states that wish to distort to a localized state, and at the same time they exhibited rotational barriers. We further considered the isoelectronic series of each π-electronic components (e.g., for π-allyl radical we considered the isoelectronic 3 electron/3-center delocalized species like H_3, Cl_3, Li_3, Cu_3, etc.) and showed that on the basis of the VB diagram promotion energy gap (G) it was possible to predict whether the delocalized species will be a stable cluster, like Li_3 or a transition state for an exchange reaction, like H_3. The G quantity increased as the binding energy of the diatomic molecule; the π-electronic components of the allylic species and of benzene fell among the unstable species. The paper was published in *NJC* in 1984, after having gone through seven referees. Not that any of them was bad, but there was a degree of disbelief in this crazy idea.

Three other things happened in the two years 1983−1984. I decided to go on sabbatical to the French laboratory established in Paris Sud (Orsay) by Lionel Salem. In the meantime, my daughter, Yifat Sela was born and she had a heart defect, from which she seemed to recover. I completed a huge review on the VB model, which I called "*The Collage of* S_N2 *reactivity Patterns*" (eventually published in *Progress in Physical Organic Chemistry* in 1985). So, while the focus was S_N2, the review gave a general scope of how to apply the model to pattern data and to make new predictions. Then Saul Wolfe came to visit us at Ben Gurion University. He was doing ab initio calculations of S_N2 reactions and wanted to meet this guy who in his own words "*calculated all the trends with a paper and pencil*". Saul was an eminent chemist and I was glad he was interested in what I was doing. In our meeting he suggested we write a book on S_N2 reactivity using the VB model and all the computational data they assembled. The enthusiasm of Saul was contagious and I found myself saying sort of a feeble "yes".

As we prepared to go to France, Yifat's doctor performed a final check up. The results were not good and he advised us to have her undergo surgery; she was 6 months old. This was heartbreaking news, and I have no idea how we managed to conduct any normal life; my wife Sara was a rock. By that time, our apartment in Beer Sheva was already rented and we lived with my in-laws. The operation was successful, and after a month our daughter was laughing, for the first time since she was born. I flew to Paris, and the plan was that my family would join me after full recovery of Yifat and after they obtained their French VISAs. We were perhaps lucky that the French were not so fast to issue the VISAs, and Yifat had more than one month to recover. We were lucky also because by the time Sara and Yifat were allowed to join me, I could already manage somehow with my French to know how to select the delicious foods Paris could offer; while until that time, the only word I knew was a *rillettes* sandwich−which means a sandwich with animal fat, which I had eaten for the whole month whenever I would eat by myself. In the meantime, I found an apartment and prepared it; it was in *Rue Massenet* adjacent to the place where the role of the French in the Suez war was planned. I also found Mme Bailly who was a *nourrice* and would take care of Yifat during the daytime for the whole year. Finally, they joined me in February 1984. This was a wonderful year in every respect.

In Orsay I already had two friends, Odile Eisenstein and Christian Minot, but I did not know all the other members of this large and world-renowned group. In my first visit to the laboratory, Philippe Hiberty approached me and said he wanted to collaborate with me on the problem of π-electrons. It turns out he was one of the seven referees who reviewed the paper, and he was both intrigued by as well as disbelieving the whole idea. I knew Hiberty's work on projection of MO-CI wave function to VB structures, and I was very happy to team with him. Philippe and his co-workers in Paris (Jean-Michel Lefour and Gilles Ohanessian) invented all kinds of ways to probe the π-distortivity of conjugated molecules. There was a lot of resistance to publishing these papers, but we somehow managed, initially in *NJC*, then in *JOC* and slowly also in *JACS*. Because we believed that science is a dialogue, we welcomed any criticism and made a habit to respond it. Every response used a new way to interrogate the π-electronic component. This initial work started an intense collaboration between Hiberty and me that continues to these days.

The year in France was exciting and full of stimulation: In addition to the π-electronic problems, Hiberty and I decided to collaborate on the VB diagram for reactivity, and try to calculate these diagrams for real reactions, using an old VB program that was written in the Orsay group by Jean-Michele Lefour and Jean-Pierre Flament, and in the years to come this activity has only intensified. I continued to develop the VB model and to apply it to more complex reactions, which were stepwise and involved mechanistic changes, such as nucleophilic vinylic substitution. I collaborated with Saul Wolfe, Dave Mitchell and Berny Schlegel, where we showed that in accord with the VB model, the gas phase S_N2 barriers correlated with the deformation energy of the CH_3X molecule. The review on S_N2 was published in 1985, and Jean-Jacques Perrier who already knew me saw it and invited me to Toulouse to give a mini-course on chemical reactivity for one month. I went to Toulouse in January 1985 in the bitter winter when even Toulouse was snowed down. The warm friendship of the Toulouse group and my excitement to give this course on VB approach to reactivity compensated for the low temperatures outside. I also gave talks in the group of Jean-Paul Malrieu and found myself in the midst of a heated (but friendly) debate with him. The French chemists were excited about ideas and I felt very welcome. I owe France a debt of gratitude for this feeling of welcome.

Late 1984, Saul Wolfe called and suggested I come to visit Queen's University, and discuss the book with him and Berny Schlegel. During these discussions it became clear that I would have to take a leave of absence from Ben Gurion University and spend about 6 months in Queens. After finishing the sabbatical year in Paris my little family and I went back to Israel for one month. Yifat, our daughter, was already chattering in

French. Soon enough we flew to Canada and arrived at Queens in April 1985. Yifat had to learn English and for a long while she would not speak to us. We were very concerned so we asked the teacher at Yifat's day care, if there was something wrong. She told us that Yifat speaks ceaselessly, and because she thinks we do not know English she does not speak to us.

Saul was a great host and he made a supreme effort that we will have the best conditions. Saul, Berny and I used to have periodic discussions. Berny and I were coming from different schools in theoretical chemistry, and these discussions were extremely important to bridge the differences and establish a mutual understanding and respect for each other's way in science. The book was initially planned to treat only S_N2 reactivity, using the computational data of Dave Mitchell, Saul and Berny, and my review in *Progress in Physical Organic Chemistry,* as a basis. The idea of a small book was reasonable and attractive. However, in that stage in my life I was in the midst of developing the VB model and expanding its coverage, so that deep down my creative urge was pushing me toward a more general treatment of reactivity. Writing a book with an inner conflict can be a nightmare.... It took me time to curb down my ambitious plan and focus on S_N2 reactivity in the gas phase and in solution. In late August 1985, Sara and Yifat flew back to Israel. I stayed one more month to complete my share of the book. It was decided that I leave all the chapters with Saul and he would finalize the book. In September, Saul and I flew to Chicago to participate in the Physical Organic Chemistry Symposium of the ACS Meeting, and subsequently I flew back to Israel. The Israeli airport in those years was small and all the family members would wait outside for their passenger to come out. The first thing I saw when I came out was the face of my two years old daughter who was held up by Sara. She saw me, and then like a flash she recognized me, and she started gasping with excitement (she did not yet speak Hebrew, and for her we did not know English). She clung to me for the next few days, as if not to let me off her sight so she will not lose me again. A week later I flew to France, and when I came back she ignored me for a few days—I was not reliable. This was a realization that my scientific work was tearing me away from my family. I had to learn the secrets of balance....

During the next six years, Saul coordinated the work on the book. He and I communicated by mail back and forth over the drafts of the book; this was not easy. But finally, Saul managed to condense the various chapters and to unify them into a coherent book. The book was published in 1992. When it came out the three authors were proud and evoked a sigh of relief.

In the period after my return to Ben Gurion University in 1985 and till 1991, I resumed my activity in all fronts; teaching general chemistry and applied quantum chemistry, working on organic conductors, further development of the VB ideas and applications to new reactions, and the behavior of π-electrons. In 1987 the department started the process of my promotion to a Full Professor, but the pace was sluggish. This changed when the textbook of Lowry and Richardson (*Mechanism and Theory in Organic Chemistry*, 3rd Ed.) came out and contained extensive coverage of the VB work that Addy Pross and I did until 1983. This made due impression and I was immediately promoted. In 1986 I got my second invitation to give a mini-course in VB theory, at the University of Alabama, Huntsville, from Sam McManus and Milton Harris. In 1987 I got the third invitation to come and give a series of lectures on the VB diagram model to chemical reactivity, this time in Lund and Gothenburg in Sweden. Per Ahlberg, Jan Sandström, and the late Lennart Eberson organized jointly this invitation. I gave these lectures only in 1989, just before the IUPAC meeting in Stockholm. This was a mini-course, which I titled: "*The LEGO Way: Curve Crossing Diagrams as General Conceptual Models for Chemical Reactivity and Structure*". My family and I would spend a few weeks in Lund and a period of two months in Gothenburg, living near the fountain with the awesome Carl Miles sculpture of Poseidon. The VB model was gaining some converts and this felt good.

The benzene story was getting its share of attention too. In 1988 I went to Switzerland upon an invitation of Edgar Heilbronner (the late) and Jack Duntiz to give The Kahlbaum Lecture in Basel and two talks in the ETH. Edgar was interested in the π-electronic ideas we published, and already while I still was in Orsay he wrote me a letter, and in his special sense of humor he let me know that he took our paper along with a few detective books to his vacation on the Swiss mountains. The ideas on the distortivity of the π-electrons of benzene were well accepted, even though they were still considered controversial. Edgar told me about his dialogue with Binsch in the aromaticity symposium in Jerusalem (1970?); Edgar asked what is an aromatic molecule, and Binsch replied "*Benzene is a perfect example*", to which Edgar responded: "*Name a second one*!"; end of discussion. In 1991, Edgar would publish a lovely paper in *The Journal of Chemical Education*, which was entitled "*Why is my molecule not symmetric*?" and this was the first positive reception of our paper. Edgar and I would publish together later on π-systems, but more importantly he impressed me by his engaging intellect and became in some ways my third important teacher in the years to come. I learned a lot from him and from his wonderful stories and quick wits.

A few events have pushed me to develop VB ideas further at that time. One was an invitation I got from Imre Csizmadia to participate as a teacher-speaker in the NATO school in Saint Feliu in 1988. I was supposed to teach a few hours and then to have a few tutoring sessions. Looking at the list of other teachers-speakers, I saw Don Truhlar, Bill Miller, Paul Schleyer, Berny Schlegel, Paul Mezey, Mike Robb, etc. It was clear to me that if I wanted to rise to the occasion; I had to develop something new. I therefore started to work out VB problems with a variable number of electrons and derive analytically all the energy expressions and the mixing patterns, something that I already started fiddling with when I was in Orsay. I ended up developing a Hückel/Extended Hückel type VB theory, and because VB theory deals with states, the scheme included effectively also the electron—electron repulsion terms. This was a lot of fun; once I figured out the rules for taking the matrix elements of VB structures and trimming them, I found that the VB structure set for a given problem mixed in Hückel or Möbius patterns, and I could therefore use simple Hückel MO programs to solve the state problems. I derived the rules of aromaticity and antiaromaticity, including for odd electron systems, and had an immediate handle on excited states. This work was written as a Chapter in the *NATO ASI* series volume C267, which was published in 1989. It would become one of the bases for the book written by Philippe and me, 19 years later.

A second motivator to develop the VB ideas further was the relationship between electron transfer (ET) and polar reactions, which has become then a hot area in physical organic chemistry. Both Addy and I wrote papers and reviews on this relationship. The late Lennart Eberson has written a monograph in which he outlined the relationship using the VB diagram model. In 1989 the IUPAC chemistry congress was held in Stockholm and one of the major topics was the ET/Polar dichotomy in organic reactions. This has diverted some of my attention to electron transfer theories and especially to the Marcus–Hush theory. Something that struck me was the outer-sphere model that was developed for distant electron transfer events, was used by organic chemists to derive the reorganization energies of many organic ET reactions. Looking at it from a VB point of view showed that there should be a strong mixing between the two intersecting states, and one could derive orbital selection rules for the ET/Polar dichotomy. During the meeting in Stockholm, Lennart and I decided to write a paper on this issue and to revise his reorganization energies that were derived using the outer-sphere assumption. For a few years later, I wrote and gave talks in which I asked my physical organic colleagues: "*Why should a transition state give up its bonding and be outer-sphere*?" Later during the years 1994–1998 (when I already moved to Jerusalem), my postdoc G. N. Sastry would investigate the reactions of ketyl radical anions with alkyl halides, and would use his "golden fingers" to show that the ET and polar processes follow different orbital selection rules that lead to different stereoselectivities and chemoselectivities and which could be predicted from the VB model of the ET/Polar dichotomy. He would further demonstrate that the ET transition is strongly bonded, and that these transition states create entangled ET-polar reactivity. The entangled ET-polar reactivity would later be verified by molecular dynamics simulation studies with Berny Schlegel and his co-workers.

The third motivation came from VB computations, which Hiberty, his students and I were doing at the time. Gergji Sini, a student of Philippe's from Albania, was generating the VB diagram for the S_N2 process, of $F^- + CH_3F$. One day I asked Gergji to see the calculations and found out that the resonance energy of the covalent and ionic structures of the CH_3F bond was huge, almost as big as the experimental bond energy. I was stunned; until that moment I believed the Pauling paradigm according to which there were covalent bonds and ionic bonds, and that in each class the corresponding covalent-ionic resonance energies were small compared with the stabilities of the dominant VB structures (the covalent or ionic) itself. Suddenly, the covalent structures in $CH_3{-}F$ were not important! What holds the bond is the resonance energy between the structures. My hunch told me this is a significant result. Philippe and I discussed the matter and decided to ask Sini and Philippe Maître, a new student in the group, to run VB calculations of a few bonds. Soon enough it became clear that some bonds, which included small electronegative atoms, had huge covalent-ionic resonance energies, even when the bond was homopolar, like F–F and O–O. We found quite a bit of experimental support for a new class of bonding, for example, the findings of Dunitz et al. of "covalent" bonds in which the deformation density was negative alongside other covalent bonds, like H–H, C–C, etc., where the deformation density was positive. Our first paper was published in 1991, but it was clear that these calculations and VB conceptualization of bonding might have just scratched the surface of a much bigger problem. Indeed, in the years to come, this idea has developed into the concept of "*charge-shift bonds*". In the beginning of 1992, Philippe would visit me for the last time in Beer-Sheva, and we would write together the 1992 *JACS* paper where we analyzed the origins of charge-shift bonding in chemistry and predicted its occurrence in the periodic table and some of its experimental manifestations. This research is still ongoing to day.

Another person I met in the Stockholm meeting who became a close friend to this day was Joe Dinnocenzo who was doing physical chemistry of organic cation radicals. Joe was a student of Mel Goldstein in Cornell and recognized me from the talk I gave in the group while in Cornell. We became friendly during the meeting and spent our lunches and dinners together in a merry company, which included Christian Amatore and Ole Hammerich, having great laughs, drinking beer and paying exorbitant prices. I decided to stop by Joe's poster, which was showing that nucleophilic cleavage reactions of cyclopropylic cation radicals proceeded in a stereospecific manner. He showed in his poster that frontier orbital theory could not make a prediction because in odd-electron reactions, two different orbital interactions were equally important, the SOMO–LUMO and the SOMO–HOMO. Because I was thinking then in terms of orbital-selection rules for chemical reactions, I immediately gave him the VB analysis of the problem; his eyes lit. We decided to collaborate and write a communication on the problem. I drafted a short paper, and Joe added all the experimental insights and even corrected some of my errors in theory. The paper was published in *JOC* in 1990; to date this is the first and only paper that derives the stereochemical rules for odd electron reactions such as nucleophilic attacks on cation-radicals and the isoelectronic radical cleavage of σ-bonds. Joe and I would publish a few more papers and would maintain a continuous communication on the application of VB theory to chemical reactivity.

In 1991 my family and I moved to our newly built house in Beer-Sheva, which shows that I had no talent for predicting my own future: the move to Jerusalem. The story started when I was in charge of the departmental colloquium. One of my invitees was Mordecai Rabinovitz from the Hebrew University, who happened to be the chairperson of the institute at the time. While we were talking, Mordecai asked me if I would consider moving to the Hebrew University. In those days, it was almost unheard of to move between universities (there was one precedent only in all sciences). In a small country like Israel there are many obstacles to such moves; everyone knows everyone else and it is not pleasant to "steal" faculty members. In fact, I was already having a flirt with the Weizmann Institute, but the President of the institute vetoed "*taking away good people from the young university*". Another obstacle was the way we live in Israel; there are not many apartments for rent and this meant that I had to sell our house in Beer Sheva and buy an apartment in Jerusalem. The price difference was 1:2 and now it is about 1:4 or more. The third obstacle was that one of my childhood friends, Avishai Braverman, was appointed President of Ben Gurion University, and the local politicians did everything to make his life miserable so he would fail and leave. A few concerned faculty members and I tried to help, and this created some emotional commitment. Despite these obstacles I was encouraged by Sara to consider the move. What helped the most to make a positive decision was the tension in the department which created around me a very negative atmosphere, and Saddam Hussein who started sending missiles to Israel on January 15, 1991. My Korean postdoc at the time, J. K. Cho, left the country immediately; my research was left in shambles. I could not do anything anyway, because most of the time we would spend in the shelters. This was the last straw; I called Rabinovitz and said yes, "*I do*". After a week or so, Rabinovitz called me, while I was in the shelter and informed me that my case passed in flying colors and what I had to do now is send him a "shopping list". It was so quick that I had no time to think; I knew that if I hedged, this might be my last chance to move in Israel. I also thought to myself that a university that could recruit so quickly must be a terrific place to move to.

Terrific it is indeed. But later when I served in recruitment committees I realized that the university was very slow and bureaucratic, “a traditional Germanic University” to use the words of Henry Rosovsky who evaluated the university long ago. I was simply lucky; the new elect President, the late Yoram Ben-Porat was a dynamic character and was driving to rejuvenate the university, and as such made many critical decisions by himself bypassing the lengthy procedures. After Rabinovitz called him, it took him a few days only to call in person the proposed referees and to give the green light for my appointment. He and his family died in a tragic car accident shortly afterward. By March 1991, I got a letter from the Hebrew University, offering me a position as Full Professor at the Institute of Chemistry. This was followed by negotiations over the conditions of the move, with the new chairperson of the Institute, Eli Grushka, and the Dean, Michael Ottolenghi. There were meetings also with the members of the Fritz-Haber Center, maybe the strongest theoretical group in Israel. The Institute of chemistry treated me with generosity; I would be a member of the department of organic chemistry and of the Fritz Haber Center, would receive startup money to buy a good computing facility, would be allowed to hire a computing specialist who would work with my group, as keeper of know-how, and so on. I was due to move on March 1, 1992. The Chairman, Eli Grushka, and the Dean, Ottolenghi, were exceptionally generous and allowed me to purchase the workstation (IBM/RISC 6000 model 550) early and use it while I was still in Ben Gurion University. At about the same time, my colleague Yitzhak Apeloig from the Technion, recommended to me his postdoc, David Danovich, who was an immigrant from Russia and had a Ph.D. in quantum chemistry. He thought David would make a wonderful computing specialist. I interviewed David in Ben Gurion University and could immediately see two features: He was highly skilled with computers and with use of quantum chemistry, and he was a very nice person, easy to get along with. So, in January 1992, when the IBM workstation landed in Ben Gurion, it was immediately put to use by Alexander Ioffe, another Russian immigrant working with me at the time, and David Danovich. I started my service at the Hebrew University on March 1, 1992, and on August 12, 1992, my family joined me, and we moved to a University apartment near the campus.

By that time I already had a small group, Chandra Reddy a postdoc (former student of Jemmis), Alexander Ioffe who used to come once a week from Beer Sheva, and David Danovich. Later in 1993 came another postdoc, G. Narahary Sastry (another former student of Jemmis), and subsequently, Avital Shurki joined the group, as my first Ph.D. student. Danovich was doing VB calculations and was the only one that could make the program TURTLE work; he was teaching the postdocs and students to do these calculations. The Indian postdocs were doing cation- and anion-radical chemistries using the VB ideas developed in past years. In 1993 I resigned from Ben Gurion University, we sold our house in Beer-Sheva to the same guy who bought our apartment and then built our house. We then bought a new apartment in Jerusalem; it was on paper still....

Sometime in early 1993, the computational needs exceeded the capability of our new workstation. A new one came on the market, the RISC 590 model, which was defined as a “super-computer”. I started raising the money to upgrade my old 550 to the new model. While I managed to do so, I realized that this is going to be a major problem in the future: how to secure state-of-the-art computing facilities at any given time. Being a member of the Fritz-Haber Center, I learned about the possibility to establish a new center with endowment from the Minerva Foundation in Germany. I also understood that Minerva would favorably regard a multi-institutional center. I naturally contacted Yitzhak Apeloig and we decided to team and submit a proposal. We needed, however, support of the idea by a few German scientists. Our natural choice was Helmut Schwarz; he and Yitzhak were good friends, and we knew each other quite well from the many conferences, and the many visits of Helmut to Israel and in particular to Jerusalem and the Technion. The second person was Lenz Cederbaum, whom I knew very well already from my days in Cornell. Helmut suggested that I write to Sigrid Peyerimhoff, one of the most highly esteemed theoreticians in Germany, and the Vice President of the DFG. So I did. Apeloig suggested Paul Schleyer who was then still in Erlangen. And finally, Helmut suggested that I write to or visit Joachim Sauer who was a theoretician in the east and was now appointed to form a theory group in the revitalized Humboldt University. I had heard of Joachim before, but I knew more about his spouse, Angela Merkel, because she did theoretical work on S_N2 reactivity and cited my work extensively, while still being in the East.

In June 1993 I visited Helmut Schwarz. This would be one of the many visits to Berlin and the establishment of long and very friendly relationships, with Helmut and his group members, especially Detlef Schröder. The Schwarz group was then conducting research on bond activation of small transition metal cationic species and accumulated quite a few puzzles. One of these puzzles was the reactivity of FeO^+ in hydrogen abstraction. I had a talk with the group members, and learnt from Andreas Fiedler, the student who was doing his Ph.D. on the topic, that he was running calculations with Wolfram Koch, and they were finding that the ground-state of FeO^+ is $^6\Phi$. Andreas further added that all his attempts to understand the reactivity of this species with H_2 failed. In the same week, I visited also Joachim Sauer. My subsequent visit to Berlin was in November 1993. I visited the group, gave a series of talks on the VB model of reactivity, and had a discussion with Helmut, Detlef, and Andreas. Helmut handed me a draft of a *JPC* paper, on the lack of reactivity of FeO^+ with H_2, despite the rosy prospects for this reaction, including the fact that it was also spin allowed. Helmut was a superb motivator, and November 20 and 21, 1993, were bitter cold days. I tried going out to see some more Berlin, but the cold chased me back into my hotel room. So, I sat in there and wrote two documents: one a draft of a common proposal to the *Volkswagen Stiftung*, and the other a draft of the paper on the reactivity FeO^+ with H_2. In the draft of the paper, I proposed that the electronic structure of FeO^+ was analogous to O_2, with a high-spin ground-state and a low-spin excited state. I further suggested that much like in the case of O_2, where the more reactive state is the $^1\Delta_g$ state, in FeO^+ with the $^6\Phi$ ground state, the reactive state is the lower spin quartet state analog of $^1\Delta_g$, which would cross the high spin state and mediate the process. Using VB ideas I could even predict the structure of the transition state. On the eve of November 21 (Sunday), the draft of the paper was finished, and I mentioned it to Helmut during the break in the concert of Maurizzio Pollini. On Monday, I presented the ideas to Helmut, Detlef and Andreas, and this was followed by an intense discussion. The paper had been improved by a few iterations, and was submitted to *JACS*, raising the option of two-state reactivity (TSR), which was further articulated in the 1995 study we published in *Helvetica Chimica Acta*. The TSR concept has started another long and close collaboration, during which time I spent 6 months in Berlin and learned to love this exciting city.

In Jerusalem, I met Yehuda Haas and his Russian immigrant co-worker Shmuel Zilberg. Yehuda was a spectroscopist who was studying the spectroscopy of benzene derivatives (and other aromatics), and Shmuel was a computational chemist. Together they found, what was known already from two-photon spectroscopy of benzene by Lionel Goodman and others, that the bond-alternating vibration mode (b_{2u}) had a higher frequency in the excited-state compared with the ground state. Shmuel Zilberg who was familiar with my work immediately thought that this must be associated with the π-distortivity model that we had been advocating since 1984. Shmuel and Yehuda wrote a communication for *JACS*. I was very excited and my interest in the problem was rekindled, I figured out a VB model, which showed on equal footing the ground and excited states of benzene and demonstrated most clearly that the reason for this phenomenon was the avoided crossing of the Kekulé structures along the bond-alternating mode. I presented it to Yehuda and Shmuel in their group seminar, and at the same time engaged Avital Shurki, then my Ph.D. student to start doing VB calculations to see whether the model was correct. She did and found it to be correct, and we published the Kekulé crossing model in 1996 in *JACS*. This has opened a new collaboration with Yehuda and Shmuel, in which we discovered that this frequency exaltation in the excited-state was a general phenomenon, and in each case could be predicted by considering the avoided crossing of the corresponding Kekulé structures; one exalted mode for every pair of structures that were made to exchange by this mode. Subsequently, Avital found an even better probe for the π-distortivity of benzene, using the excited-state geometry of distorted benzene derivatives, which were made by Jay Siegel. She showed that while in the ground state these molecules exhibited strong bond alternation, the $\pi\pi^*$ excitation eliminated the bond alternation and led to a molecule with uniform C−C distance. Thus, one of the central beliefs that the D_{6h} symmetry of benzene was due to its delocalized π-electrons was proven to be wrong.

In the meantime, our German friends received the idea of a Minerva Center for Computational Quantum Chemistry very well and both I and Yitzhak managed to recruit prominent Israeli scientists who would join us as members of the center in the two institutes. Sometimes later, in December 1994, I wrote the first draft of the proposal and sent it to Yizhak. When the draft was complete, we sent a copy to the vice president for research and development at the Hebrew University; we knew that the competition was rough and tough, but we hoped to succeed and win the grant for establishing a center. In 1995, there was a Berlin-Jerusalem meeting, organized by Helmut. In the eve of the first day, Charlotte Goldfarb, who was the world expert on scientific relationships between Israel and Germany came to visit us. She was stationed in Bonn and came to see me after having a look at the draft of my proposal. She poured cold water on my enthusiasm and showed me all the faults we made and the naivety of our proposal, not knowing the *modus operandi* and what really counts in Germany and for the Minerva Foundation. I took her admonition to heart and when I went back I sat down and discussed her suggestions with Yizhak, and we both agreed that she was right. Finally, the Minerva proposal was submitted in early March 1995.

On May 3, 1995, Helmut notified me that I was awarded the Lise Meitner-Alexander von Humboldt Senior Award, which meant that I had to spend six months in Germany. In August 1995 my family and I left Israel on our way for a sabbatical year in Rochester University, mainly to work with Dinnocenzo on cation radicals and teach a VB course in his department. Other than the maddening weather, this was a very productive year for me: During this time, Yehuda, Shmuel and I completed a short review for *Accounts of Chemical Research* on the Kekulé-crossing model for π-systems. The late Lennart Eberson, Bjorn Roos and I teamed on a paper that tested the VB model predictions on the reactivity of nucleophilic substitution of odd-nonalternant hydrocarbon radical cations. Dinnocenzo and I formulated a VB model that can predict the structural patterns of σ-cation radicals. More stuff was coming out on charge-shift bonding, and on bonded ET-transition states. Most importantly, I prepared an extensive course on VB theory, which would serve me in the future.

In the middle of 1996 I was notified that the Minerva grant to establish a center for computational quantum chemistry was awarded to Apeloig and me. My family and I left Rochester in August 1996 and went back to Israel. Our apartment was not yet ready, and we lived in a rented university apartment. Finally, in early September we moved to our new apartment, and already in September 5, I had to fly to Berlin to start the Alexander von Humboldt fellowship award. I left not knowing even my home address, and coming back the taxi driver asked me where to take me, and my answer was that I was not sure what my precise address was, which caused him to give me a diagonal look that is reserved for strangeness.

I stayed two months in Berlin and enjoyed the rich culture of the city and its cosmopolitan flavor. I traveled to a few places in Germany (Marburg, Essen, Würzburg, Munich, Köln, Bonn, Heidelberg, Gotingen etc.) and gave lectures about VB and reactivity, about the π-electronic theory, TSR, and the extensive work Danovich and I did on spin inversion in the reaction $FeO^+ + H_2$. Helmut and I discussed the future of the center and how it should run, and his interest in the reactivity of FeO^+ as a model for the active species of cytochrome P450. Each time I would see Helmut, he would ask the same question: "*And what about P450*?" There were many interesting results on P450; there was the rebound mechanism of Groves that suggested the presence of radical intermediates, there were the results of Newcomb, who showed controversial data that ruled out the rebound mechanism, and there were the kinetic isotope effect (KIE) studies of Dinnocenzo and Jones that supported the rebound mechanism. What was right? What was wrong? I knew about these controversies and their KIE results from Joe Dinnocenzo and Jeffrey Jones, when I was in Rochester on sabbatical. I was reluctant initially to handle P450, because first, I did not understand the active species, and it was not clear to me if it had really a relationship to the small FeO^+ reagent. After a concentrated effort, I managed to reconstruct the electronic structure of Cpd I of P450, and to recover the two-state nature of the reagent, but these were degenerate ferromagnetic and antiferromagnetic states of three unpaired electrons, one residing on the porphyrin, the other two on the FeO moiety. I prepared a rough draft of a paper, and after many rounds, it was completed in July 1997 during the inauguration of the center in Jerusalem.

Detlef and Helmut were in Jerusalem in July 1997, because the center was inaugurated at that time with an international conference, including the members of the center and many guests. The center was named as *The Lise Meitner−Minerva Center for Computational Quantum Chemistry*. I was appointed the Director of the center and Yitzhak Apeloig as co-Director. Helmut Schwarz was appointed as the chairperson of the scientific board of the center (in German: *Beirat*). In addition to Helmut, the other Beirat members were Sigrid Peyerimhoff, Joachim Sauer, Eli Grushka, Nimrod Moiseyev, and Addy Pross. As Director, I had to organize almost every year-to-a year and a half a conference that would present the work of the members and would bring in guest speakers from other countries.

The P450 paper (that was eventually published after many tries in *Chemistry A European Journal*) and the establishment of the center would define a new phase in my scientific activity, which stretches from 1997 till this day. The center enabled us to purchase a computing facility that was updated every year and lasted in a state-of-the art form till 2003. We had money for guests, small grants to members, awards, conferences, etc. But above all, the sheer existence of the center has served as a seed to raise more money. I, for example, had from 1997 on several active grants, which gave me the means to increase my group and to do more extensive scientific work. Another goal that the center fulfilled was the establishment of a quantum chemistry school in Israel; a school that was sorely missing in view of the otherwise very strong theoretical chemistry in Israel. I also became extremely busy, having a large group, a serious administrative duty and a secretary. I lost my freedom forever, but in retrospect I gained a lot in return.

In 1997−1999 I hired a few excellent postdocs; Michael Filatov, John Galbraith, Nathan Harris, and Wei Wu. Michael Filatov came from Walter Thiel and was a DFT expert who did methodology and application. Wei Wu was a skilled mathematician who wrote a VB program all by himself. Johnny Galbraith was a student of Schaefer, with excellent computational background and with a passion to work in VB theory. Nathan Harris, formerly a postdoc of Koop Lammertsma, who came with a Fullbright Fellowship was a superb computational chemist with immense patience and perseverance. In addition, I still had Avital Shurki as a Ph.D. student, and I admitted to the group a few undergraduate students, among them Shimrit Cohen who would later become my Ph.D. student.

With Wei Wu, David, Avital and Johnny we had a critical mass to form a VB subgroup that investigated bonding and reactivity; Avital looked at charge-shift bonds, Johnny was doing transition metal hydrides, while David and Wei were looking at no-pair bonding of ${}^{n+1}M_n$ species, where M is a monovalent atom, like Li, Cu, etc. This type of bonding did not require electron pairing, but in fact, all the electron spins were aligned in the same directions, and the bonding was sustained by covalent-ionic resonance energy of the high spin VB structures. Using VB calculations for the triplet state of the ${}^3Li_2$ dimer, which was very weakly bound (less than 0.5 kcal/mol), we were able to construct a simple analytic VB model that predicted the binding energy for any cluster size. The interaction energy grew very quickly and converged around 10−12 atoms; years later in ${}^{n+1}Cu_n$ the bonding energy per Cu atom reached as much as 19 kcal/mol, without any electron pair. This was very exciting. With Wei being around, we developed during these years a semiempirical VB method, with DFT input, so-called VBDFT(s), and a nonempirical VB-DFT method (the latter is ongoing).

With Michael Filatov, Nathan Harris and Shimrit Cohen we could start DFT calculations of P450. These calculations were painfully slow then, but nevertheless, the results enabled to treat pieces of the reaction mechanism of alkane hydroxylation by P450; we published these papers in 1998 and 1999 in *Angewandte Chemie* and thereby laid the foundations for TSR in P450. Michael Filatov developed also DFT methodsn (ROKS and REKS) for treating open-shell systems with more than one Kohn−Sham determinant, and akin to VB theory.

The full P450 treatment had to wait to 1999, when François Ogliaro, a former Ph.D. of Saillard and a postdoc of David Cooper, joined us, and augmented the P450 team. Initially, with guidance from Nathan and then independently, he undertook, even if somewhat reluctantly at the beginning, the study of the full mechanism of alkane hydroxylation by P450. We started with methane as a model alkane, but what we found then is a still viable model for the TSR paradigm in P450 reactions in general. We found that the quartet (ferromagnetic) and doublet (antiferromagnetic) states of the active iron-oxo species, so-called Compound I (Cpd I) performed hydrogen abstraction, at almost equal energy barriers, leading to the formation of weakly coordinated alkyl radicals/iron-hydroxo species. Subsequently, the two surfaces bifurcated: the quartet state process encountered an additional barrier for the formation of the ferric-alcohol complex, while the doublet state process was barrier free. This excellent work of François, which clarified many of the major puzzles and controversies in the field, was published in 2000 in *JACS*. It started us in the P450 field in a major way.

In 1999, I visited Berlin for the last portion of my Alexander von Humboldt Award. In that year and in the previous one, Yitzhak Apeloig and I coordinated our stays and had a lot of fun being together in Berlin and having in addition the company of Helmut whenever his feet would touch the soil of Berlin back from his many, many trips. I brought with me my usual set of talks and added on P450. Of all the selection, the P450 story was the star, everywhere I went (including Germany, France, London, and Switzerland where I went twice as a Trosieme-Cycle Lecturer). In the same year, the WATOC conference was held in London. I gave a talk there on P450, which was well received by the audience; theorists liked it when theory can be used to make order in such a complex system. After my talk, Walter Thiel, who was then still in Zürich, suggested we collaborate on this topic using the QM/MM method he was developing then. Walter and I had known each other for a few years, and we seemed to complement one anther and to get along extremely well; we still do. I of course agreed, but it took two years to consummate the collaboration. When I returned from London, our spouses, Zippie and Sara, joined Yitzhak and me and we decided to tour the eastern part of Germany at the finale of the Humboldt award. On the way back to Israel I took with me two loaves of the delicious local bread.

In the meantime at the end of 1999, Sam de Visser, a former postdoc of Mike Robb, joined my group. His start was sluggish, but very soon he blossomed and became a highly productive and reliable postdoc. Furthermore, Sam was a very patient and dedicated teacher and he took charge of educating many of the undergraduate students who were in the group. He and François got along extremely well and started collaborating and producing together first-rate work and lots of it. Then Pankaz Sharma, a former postdoc of Jemmis, joined the group, followed by Jose Kaneti, from Bulgaria, and Shimrit Cohen who has started her graduate research. The P450 team grew significantly. Initially, François looked at the effect of bulk polarity and amidic-type hydrogen bonding to the thiolate ligand of Cpd I and found that the electronic structure including the Fe−S bond distance were undergoing large variations compared with the gas phase; it was then that we started calling Cpd I "*a chameleon species*" that adopts itself to the environment that accommodates it. Then with a team effort lead by François, we looked at a bigger model system and showed that Cpd I was behaving like a chameleon also for this larger model system. Subsequently, in a pure thought "experiment", Sam took the lead and, with François and Pankaz, he showed that this feature of Cpd I carried over to its reactivity-selectivity in C−H hydroxylation vs double bond epoxidation. Later when Devesh Kumar would join, he and Sam would extend the notion to the effect of electric fields on regioselectivity of P450 oxidation. The results of these thought experiments were very exciting, and we are still pursuing this idea.

In the year 2001, David Danovich, François Ogliaro and Shimrit Cohen traveled to Mülheim to learn QM/MM, by interaction with Walter Thiel's student Jan Schöneboom and his postdoc Natalie Reuter. It was decided to look at Cpd I of the enzyme P450cam, which is a bacterial enzyme that hydroxylates camphor. To our satisfaction, the QM/MM results supported completely the conclusion of the model system that Cpd I behaved like a chameleon species and accommodated his electronic structure to the protein environment of the enzyme. The paper, which was published in *JACS* in 2002, was as far as I know the first QM/MM treatment of a complex metalloenzymatic species. In 2006, an experimental paper by Brian Hoffmann, John Dawson and co-workers would verify the results of these calculations, using the analogous enzyme chloroperoxidase (CPO). Subsequently, the QM/MM investigations of Jan Schöneboom and Shimrit Cohen, recovered fully the TSR mechanism of camphor hydroxylation by P450cam. This compatibility of a carefully chosen model system with a complete treatment of the species in its native protein environment was encouraging. So, in the next years we continued to use a blend of model calculations and QM/MM treatments. The collaboration between Walter's and my groups has been intense to this day.

When François left the group, another postdoc, Devesh Kumar, a student of Roychoudhury, joined us in 2002. Devesh came from a background of physics from Gorakhpur University, and it took him a year to acclimate, but when he did, he became a powerful addition to the group; he loved big and complex molecules, and he and Sam forged a very good mini-team. In the years 2003−2007 a few more students and postdocs joined the group: Sebastian Kozuch and Elina Ploschnik started in 2003 as M.Sc. students, while Dan Fishelovitch started his Ph.D. in 2005 and is a shared student by me, Ruth Nussinov (from computational biology in Tel Aviv University) and Chaim Wolfson (from Computer Sciences in Tel Aviv University). In the same year, I had two Israeli postdocs: Carina Hazan, a former student of Chaim Gilon, and Ronen Shacham, a former student of David Avnir and Dani Mandler. Rouslan Kevorkiantes, a former Ph.D. student of Walter Thiel joined us in 2004. Then came Etienne Derat, a former student of Stephen Humble, who himself was a student of Hiberty, so this makes Etienne Hiberty's "scientific grandchild". Etienne was followed by Hajime Hirao, a former student of Hiroshi Fujimoto; Kyung Bin Cho, a former student of Per Siegbahn; Maria-Angels Carvajal, a former student of Santiago Alvarez and Juan Novoa; Yohann Moreau, a former student of Xavier Assfeld; Hui Chen, a former student of Shuhua Li; and Yong Wang, a former student of Keli Han; and Nihar Jena, a Physics student from Mishra from Banaras Hindu University. By and large all were competent and highly skilled young people.

This growth of the group has resulted in consolidation of the TSR concept in P450 chemistry and has extended it to other areas. Initially, Sam and Pankaz, then Devesh and subsequently Etienne, Hajime, and Chen have extended the TSR concept to the chemistry of polyoxometalates in collaboration with Ronny Neumann from the Weizmann Institute, and to the chemistry of the nonheme iron-oxo made by Larry Que, Wonwoo Nam, and others. Following the work of Chunsen Li from Wei Wu's group, which started collaborating with us on P450, Kyung Bin, Devesh and Yohann extended the TSR concept to understand the phenomenon of KIE jumps. Subsequently, Etienne and Yohann started a collaborative project with Carsten Bolm on the azo analog of Cpd I, and then teamed with Chen and Hajime and further extended the concept to amidation and aziridination process. Hajime was also developing his own ideas in method development and I, remembering the gesture of Nick Epiotis and the way Roald treated me in a similar case, encouraged him and let him publish on his own. I would later treat similarly my student Sebastian Kozuch, who developed a pretty model to treat catalytic cycles; in his first completely independent paper I added the asterisk by his name.

Sam and Devesh initiating and teaming with Pankaz, Rouslan and Hajime treated model systems of horseradish peroxidase (HRP) and heme oxygenase (HO). With the arrival of Etienne, who loved QM/MM and complex systems, our local QM/MM activity intensified. Etienne was the first in the group to treat a heme enzyme other than P450 with this method; this was active species of HRP. One of his studies, on the oxidation of ferulic acid by HRP, exposed us to the proton coupled electron transfer (PCET) mechanism, which is utilized by enzymes to oxidized remotely docked substrates. His work on the activation of hydrogen peroxide by HRP lead us to collaborate with Carme Rovira and to "discover" the wonderful role of water as a unique "bio-molecule". He and Kyung Bin started looking at nitric oxide synthase (NOS). Kyung Bin was already conversant in NOS chemistry using model systems, so after Etienne's departure he took over the project and formed a mini-team with Maria; they are still working on NOS. Following the initial model studies by Devesh, Etienne and Yohann have teamed to do QM/MM calculations of HO, and latter in 2006 transferred the project to Hui Chen. Etienne has begun also looking at CPO, and tutoring Chen who has been engaged with this project to this day. Chen has started looking at myoglobin (Mb), in collaboration with Masao Ikeda Saito. Dan was doing with Carina studies of the human P450 3A4 enzyme. In 2007, Yong who just joined us and had a background in P450, started working on a fascinating P450 StaP enzyme, in collaboration with the group of Shingo Nagano from the RIKEN Spring-8 Center in Hoyogo. In P450 StaP we showed how a P450 enzyme could attain a peroxidase-like activity using strategically placed residues and the nimble biomolecule, water, leading together to PCET activation of a remote substrate. Enzymes are complex and hence bags full of surprises. Each enzyme has taught us something new....

The area of oxidation chemistry of enzymes and synthetic reagents has inherent complexities irrespective of the size of the molecule, and in my experience the interplay of theory and experiment in this field is almost a must. I have been fortunate in this sense to interact very strongly with experimental groups from the start (Helmut Schwarz and Detlef Schröder). I regularly consulted with my experimental colleagues, with Dave Ballou, Carsten Bolm, John Dawson, Joe Dinnocenzo, Jay Groves, Fred Guengerich, Masao Ikeda Saito, Jeff Jones, Paul Ortiz de Montellano, Wonwoo Nam, Shingo Nagano, Marty Newcomb, Ronny Neumann, Hiroyasu Onaka, Tom Poulos, Larry Que, Steve Sligar, Ilme Schlichting, and Wolf Woggon. With some of them I collaborated, and this experience has been immensely enriching.

Before I end this story, let me add that throughout this adventure with enzymes, I had a dream; to be able to one day apply the VB diagram model to the reactivity patterns of P450, and to use VB theory to understand bonding in these enzymes. This dream has been realized recently, when Sam, Devesh and I completed a VB treatment of alkane hydroxylation by P450 and showed that VB theory leads to understanding of the key mechanistic features and enables one to predict barriers for the hydrogen abstraction step (*JACS*, 2008). In another paper, Chen and I showed that by the CASSCF/MM wave function of oxy-myoglobin can be transformed to a VB wave function and lead thereby to a lucid picture of the Fe$-$O$_2$ bonding (*JACS*, ASAP). This combination of enzymes and VB theory closes a cycle for me.... Another closing of a cycle was the book on VB theory, which Hiberty and I put together in a frenzied activity in 2007. Furthermore, the dealing with enzymes has finally made me courageous enough to start thinking how to treat brain chemistry. I hope I can contribute in the future to this exciting field, and if not, then at least to learn something new. In a sense, I am happy to be again a student.

Sason Shaik

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