Face to Face

This section features conversations with personalities related to science, highlighting the factors and circumstances that guided them in making the career choice to be a scientist.

Leading a Full Life in Two Worlds – Arts and Science!

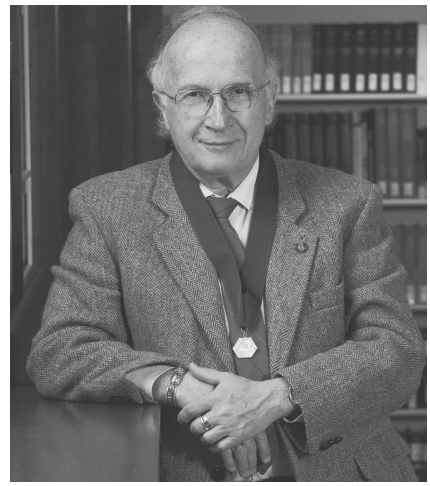
Roald Hoffmann talks to K L Sebastian

Roald Hoffmann is the Frank H T Rhodes Professor of Humane Letters Emeritus at the Cornell University, who has made seminal contributions to chemistry, for which he was awarded the Nobel Prize in the year 1981. He was born in 1937, into a Jewish family in Zloczow, a small city in Poland. During the Second World War, his family had to live in a labor camp. After escaping from there, they hid in the attic and storeroom of a local school for eighteen months. They migrated to the US in 1949. Hoffmann studied at Stuyvesant High School, New York, and then did his Bachelors at Columbia University. He continued at Harvard, earning a Masters and PhD from there. His supervisors for the doctoral degree were Gouterman and Lipscomb (who won the Nobel Prize in Chemistry in 1976). Under the supervision of Lipscomb, Hoffman and Lohr developed the extended Hückel method, which was immediately applied to a large number of problems in chemistry. Aided by the method, Hoffmann and the well-known organic chemist R B Woodward (Nobel Prize winner in chemistry, 1965) developed the very important Woodward–Hoffmann rules, which are well-known to all students of chemistry. Another important contribution is the concept of isolobal analogies. He is unique in that his interests in the arts match his interests in chemistry. He has published five books in poetry and is very active in literary circles. In his own words, he is "trying to lead a full life, in and out of science". Interested readers may find out more about him at http://www.roaldhoffmann.com. Here is a brief interview with him.

K L Sebastian

KLS: Your very early childhood was in Poland, under the Nazi rule. What are your memories of that period?

RH: I was two-years old when the war broke out, four when darkness descended on us with the Nazi invasion, seven when the war was over. It is hard to tell apart what I remember from what my mother told me. I do remember word games and geography in the attic where we were hiding.



I remember my mother trying 'cupping', with old jam jars on my uncle who came in sick from the forest. I remember looking out, and seeing children playing in the schoolyard, for we were hiding in the attic of a school-house. I could not play with them.

KLS: During that period, your mother essentially taught you. What all subjects did you learn and what interested you the most?

RH: I loved geography, and still do. She would ask me how I would get from where we were to San Francisco, and I could not skip the name of any body of water we passed.

KLS: Tell me about your schooling. Was there any particular teacher who had a strong influence on you?

RH: None really till college at Columbia. And then the world opened up to me in the arts and humanities – to have Mark van Doren in a poetry course, Donald Keene for Japanese literature, Martin Ostwald to tell us of Greek drama, Howard McParland Davis in the story of Italian Renaissance art! It was only in my last year there that I came upon chemistry courses that stood out – an introduction to chemical physics by George Fraenkel, a course in statistical mechanics by Ralph Halford.

KLS: When did your interest in chemistry start? How good were you as an experimentalist? When did you get interested in theoretical chemistry? What were the reasons for this interest?

RH: I played with chemistry sets, and read of Marie Curie and George Washington Carver. But I became a chemist almost by accident. Good research experiences at national laboratories made up for routine teaching. I worked up my courage to tell my parents that I did not want to become a physician, but I did not have the courage to tell them I wanted to be an art historian. I went to the Soviet Union on an exchange after two years of graduate study in chemistry at Harvard; I think that may have been an attempt to avoid a decision. I committed to chemistry ¾ of the way through my PhD in chemistry.

Theory came from those two Columbia courses, and from a feeling that I was not good as experimentalist.

KLS: When was the extended Hückel theory developed? Tell us about the development of the

extended Hückel theory, and its impact on chemistry at that time.

RH: Well, it was developed in the Lipscomb group, coming out of approximate MO studies he had done, and his group tooling up for so-called ab-initio calculations. We were influenced by Mulliken, by a paper by Longuet–Higgins and Roberts. I came up with a simple vector decomposition formula for calculating overlaps. Larry Lohr and I, helped by Dick Stevens, programmed the first extended-Hückel-like programs in Fortran for the IBM 604s just becoming available.

For a while, perhaps 2 or 3 years, it was the only approximate MO program available. Quickly overtaken by CNDO-type methods and HF-SCF calculations, it nevertheless fitted my desire to understand, my willingness to accept quantitative inadequacy. And it positioned me to be able to calculate any molecule in the world, any. And so allowed me to rise to Woodward's challenge of computing electrocyclic reactions and cycloadditions.

KLS: In your younger days, did you have any scientist whom, you wished to emulate?

RH: Perhaps Marie Curie.

KLS: Tell me something about your love for molecules. How did it start?

RH: First, it came from Lipscomb introducing me to boron hydrides. What wonderful complexity! And we worked on the carboranes, which showed me three-dimensional isomerism. The orbital symmetry story led me into organic stereochemistry, which I just loved. And that you could tell the course of a reaction from the isomers observed – that was astounding,

KLS: Tell us about how you came to develop the isolobal analogy.

RH: I saw pieces of it, done by other people – by Wade and Mingos for polyhedral magic electron counts, by Halpern for d^8 complexes and carbenes. But I think the real preparation was that I knew very well the orbitals of pieces of organic molecules – CH, CH_2, CH_3. And I could see how you could build up the denumerable infinity of the organic universe from these. So Mihai Elian and I looked at inorganic pieces, ML_n fragments. And I all of a sudden saw how they were patently related to organic building blocks.

KLS: Would you like to share any specific incident, which had a big impact on your career?

RH: I think doing the extended Hueckel calculation on two ethylenes interacting, seeing the level crossing, seeing how different it was from the correlation diagram for a Diels–Alder reaction – that had a tremendous impact on me.

KLS: You have made huge contributions to chemistry. Could you name a few that you consider as the most significant. If possible, elaborate on them.

RH: You have named the extended Hueckel method, the isolobal analogy. And I have added the orbital symmetry story. I would further add our explanation of the splitting of lone pairs or radical lobes a certain number of bonds apart, what we call through-bond coupling – that felt wonderful to understand. Also being able to understand band structures in detail from the same perturbation-theory based ideas that I used for molecules was significant. Teaching solid state chemists not to be afraid of solid state physics, I count as a major achievement.

KLS: In your opinion, what is the most significant development in chemistry over the last five decades?

RH: I think the advances in nuclear magnetic resonance and X-ray crystallography.

KLS: You have been a very successful researcher for more than five decades, and you continue to be very active. What is the secret?

RH: And you know I have had distractions. Such as writing. Still the next molecule in a journal remains a joy. Even if I didn't predict it. I think the key is this poetic concentration on the detail of the real world – if I understand this molecule, and I most certainly want to, I will understand the world.

KLS: You have had several collaborators worldwide, and have been a source of motivation for a large number of scientists, worldwide. What motivates you the most?

RH: I continue to be amazed by the variety of molecules, their shapes and properties. The assembly rules seems simple (like the tetravalence of carbon), yet matter itself pushes against the rules (as in electron-deficient and -rich molecules). What motivates me is trying to understand shapes, reactions, colors. With the certainty of not being able to understand them all, and a peace with that partial success.

RH: Getting a relative simple qualitative explanation gives me the greatest pleasure.

KLS: What are the things you like the most in academia? Are there any dislikes?

RH: I like teaching, which I no longer do. I miss it. I like it that I learn from teaching how to explain things. That I learn from it how to speak to diverse audiences.

KLS: Everyone talks about indices like h-index. You yourself have a very high h-index! What is your opinion on using these to judge the abilities of a scientist?

RH: They are a measure, an imperfect one. I have a general resistance to single indices – they cater to the human predilection for simplicity, when the world is complex, and beautiful for that complexity.

KLS: I know that you have written poems, and have been keen on theatre. Tell me about your interests and activities.

RH: A recent autobiographical play, '*Something That Belongs to You*', has just been published. But performance is more important than publication in theatre, and performances are hard to get. Poetry is very important to me, mine and that of others. I have just edited a translation (by others) of Joy Goswami's Bengali poems. In poetry words build worlds; I love the English language, I love the tension and meaning that words juxtaposed in the right way can create.

KLS: Did you ever think if you were not a scientist what career path you would have considered?

RH: I think I could have well been an art historian, a path that attracted me in university years. But also I could imagine myself as a full-time writer. In another world, I would even try fiction, which I have not done.

KLS: You have visited India many times. What are your impressions?

RH: India has always struck me as vibrant, alive. The approaches to Howrah Bridge in Kolkata may seem like hell to some, but I see life, people scrambling to make a living. I love the music, ever since my old friend Swaminathan, introduced me to it, of all places, when we were both for a year in Moscow, oh so many years ago.

KLS: What would be your message to the young researchers, starting their career, especially in countries like India?

RH: Enjoy that molecular richness which gives me pleasure to this day. And try to understand, a pleasuring of the mind in the end. And to be shared with others through teaching.