

# Early Ideas in the History of Quantum Chemistry

## Karl Jug



Born in 1939. Studied physics in Frankfurt (Main), Germany. Did his thesis under Hartmann in the field of molecular physics in 1965. Postdoc with P.G. Lykos, 1971 guest-prof. at Johns Hopkins (at R.G. Parr). Assistant and Associate Professor in St. Louis, USA, from 1969-1975. Since then Professor of Theoretical Chemistry at the University of Hannover where he developed his [SINDO-Method](#).

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<a href="#">Video clip</a>	Jug talks briefly about SINDO	DivX; 5 MB	Just in case, for Win9x,ME,XP: Get the free download player from <a href="#">DivX-Company</a> . . Or you may use Microsoft Media Player 9 or 10, after having installed above the Divx Player (which also installs the codecs) : <a href="http://www.microsoft.com/">http://www.microsoft.com/</a> . .	in German
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## Interview with Professor Karl Jug (*in English*)

Hannover, Univ., Institut Theoretische Chemie, 18. Nov. 1998; 14:00

**Dr. Anders:** Professor Jug, thank you very much for the time you reserved for this interview. You are director of this institute as well as editor, author (1) and co-author of articles in books and in well-known journals, some 200 to this date, if I count correctly. So most certainly you are a very busy man. In order to start abruptly with the interview I would like to ask you in which year you were born.

**Professor Jug:** In 1939.

**A:** This means that you belong to the second or third generation of quantum mechanics or quantum chemistry.

**J:** True, this is correct.

**A:** How did you come to quantum chemistry and where did you learn your quantum chemistry?

**J:** I am a physicist and have studied in Frankfurt. It was more by coincidence that I had a class in physical chemistry in the first semester taught by Hartmann (2), a topic which was difficult for beginning chemists; no wonder since it was intended for third and fifth semester students. On the basis of this physical chemistry course I tried to learn general chemistry which ran parallel to it. Hartmann had his lectures at that time already strongly 'mathematized'; he had introduced things which were very unusual at that time, the residue theorem of function theory for example. That has attracted me strongly as a physicist, particularly since I had dealt in earlier already with function theory and thus had an easier access to these ideas. And as I then began, approximately in the seventh semester, to think about what to do in the near future, I had actually something else in my mind such as nuclear physics or theoretical physics. And then - -

**A:** When was that?

**J:** That was around 1961 to 1963. There I started to think how I should continue. I did therefore actually all lab work available in physics, more than required. Only to finally wind up with the conclusion that all this was not so very interesting. And the colleagues in theoretical physics were partially already again busy moving to other universities or came - for example Greiner (3) who had just arrived at Frankfurt - when I had already finished. And Steinwedel was there, Süßmann, Beck.

But - I must say, when I heard that one could, as a physicist, do a diploma thesis also with Hartmann (chemistry faculty), covering molecular theory, then I thought that this could be of interest to me. I thus went to Hartmann, that was in 1963, I was in the eighth semester, and I asked him whether I could also do this kind of work. He gave me two areas to choose from: one statistics, which was the Ising model (4), but of which the others had already warned me, and molecular physics, which in those days was still being called

'molecular theory'. So I told him that I would rather like to do work on molecules than on anything else.

And this decision turned out to be quite right. I was thus given the book of Ballhausen which had just been published, his Ligand Field Theory (5). Hartmann told to me: If you have read what you want to know, then come back. After one week I returned - I had gone half way through the book and I wanted to begin my work. But at that time in physics, as is true in part also nowadays, there was no time limit for this type of work. By the way, presently here in Hannover, in chemistry a master's thesis takes about six months. But, as I said, in physics in those days time spent on a master's thesis was not limited and there were some students who worked on their diploma thesis for many years.

Now, I was a bit lucky, because in this institute there existed a Zuse machine (6). That was the only computer which existed at the University of Frankfurt at that time. Concerning such matters Hartmann had always been quite foresighted. Anyway, so I worked on a titanium complex - transitions, spectra - which was something well-known and well understood. But I was supposed to do it somewhat differently, with approximated functions from a particle in a box model (7). The electron interaction was also to be considered. Unfortunately it soon turned out that one needed products of four Bessel functions and that one had to perform a double integration over them for which there were no formulas in the literature - I had to derive new formulas for some of these integrals.

In order not to spend too much time on my master thesis I had to switch at some point to numerical mathematics. The Zuse machine however was insufficient for this. I had to go to Mainz (50 km from Frankfurt - *Interviewer's note*) instead. I had to work nights at this university from 8 at night till 8 in the morning, a time when nobody else needed the machine. One had to operate the machine all on his own. So there I stood and pushed some buttons to start the thing (the so called bootstrap loader which had to be loaded by hand: bit by bit, byte by byte - as was the standard procedure in a time when there were no startup EPROM loaders I's. n.). But it worked. I went there a few times and I could finish my master thesis (8).

**A:** Excuse me - which computer was that?

**J:** That was already a small IBM machine. I still calculated in ALGOL (9). At that time ALGOL was the language of choice, which was a bit better than this FORTRAN II (10). There I had to use *punched tape*, not *punched cards* which were used only later. The handling of these punched tapes had to be done with extreme caution in order not to tear them since a part of one's work would be lost - one could not glue the tape in any way, one had to redo the whole job. Well, that was then all still pretty primitive . . .

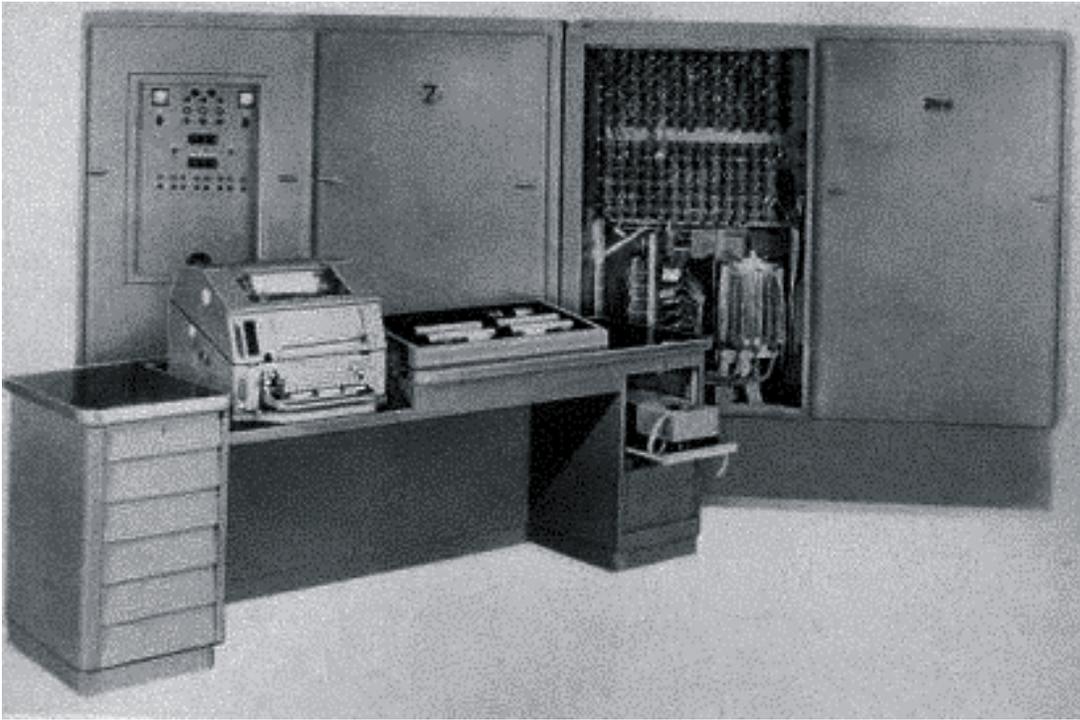
The Zuse was of course huge in its dimensions as compared with today's computers. It was "standing freely" and was as large as a small closet, at least 2 m long, 1 m wide and about 1 meter high. At the height of a table there was a board for the console elements and where one could also sit and write, taking notes and similar things.

**A:** Assembler level or on which level was that?

**J:** Assembler or ALGOL. But I have used only ALGOL

**A:** What type of Zuse was that?

**J:** I don't recall that for the following reason: For Hartmann this kind of work was only of secondary importance, one has to state this quite clearly. He belonged to a generation which had not learned any theoretical chemistry, let alone computer applications. Although he was very generous in procuring the means, he had no high esteem for computers. Those who wanted to work with such a machine were supported by him. On the other hand it was not appropriate in those days to point out one's programming achievements, and in this sense I had done nothing special, at least not while I was in Frankfurt. There were only very few people who were occupied with the underlying theory and who had programmed something more general. We wrote programs to solve our specific problems, nothing beyond that. Those were no universal programs, they were connected to a certain goal and of course they had lost their purpose once the work was finished.



**A:** Unfortunately there are nowhere old programs to obtain or people don't want to show them. I cannot find a single old FORTRAN or ALGOL program. Do you still have old print-outs?

**J:** The fact is: Later, when I did my doctoral thesis in Frankfurt and in Darmstadt (*Germany, 30 km south of Frankfurt – l.n.*) I had calculated in ALGOL. There at Darmstadt was a larger machine, actually an IBM 7090, which was already a fairly large and comfortable machine (11). But when I arrived in the USA, ALGOL was already no longer in use and I had to rewrite everything into FORTRAN. This was done on punched cards which I kept in huge boxes which I always had to carry along. That was really a large amount of punched card, maybe 3000 in the end. Those I even brought with me here to Hannover (Germany) when I returned from the States later on. But after another ten years of storage I said 'finished'. And then these cards were solely used for taking notes. We still have a great many of them.



In the basement we also have these old programs, that was FORTRAN IV (10), maybe the last ones even in FORTRAN V. (12). dating from the times in Hannover. But from the very first days unfortunately nothing has been saved. Also the punched tapes, which I mentioned previously, do no longer exist - one can no longer reconstruct that. Most likely I would also have difficulties to consider whether I still have print outs of these old programs somewhere; I wrote them once of course - but the print outs most likely have been lost.

**A:** That's a pity. One of my starting ideas as to put these original programs in storage, keep them, make them available. That's too bad - a piece of history lost forever.

**J:** Yes, but recall that 35 years have passed since then.

**A:** Yes, of course. But for somebody who wants to write about history this is regrettable. For they are the early stages in the history of quantum chemistry which I want to bring to life again, or at least to describe it, beyond the documents in the literature. Further question: How was the mood in the 70's when I wanted to work with Fraga (13).

**J:** Yes, Fraga was a well-known man at that time.

**A:** Yes, but finally I became an analytical chemist because of job perspectives and I became interested in the cleanliness of the water of Lake Constance.

**J:** In the theory we are now approaching this reality, we come closer to many practical applications. It took a long time, but in earlier days we simply proceeded in a too puristic way. There were questions concerning solutions of mathematical questions which were only loosely connected with chemistry. But the real chemical questions were only occasionally treated and then also only in a very approximate manner. Maybe spectroscopy was a part well covered, still stemming from Huckel's times, and later on the structures of molecules. But in the course of time many things have been changed.



PICTURE IBM 7090

**A:** How was the mood then, in the beginning of the 60's.

**J:** It was very optimistic. When I started with Hartmann there existed already a fairly large group. These were mostly people who were older than I was and who had not had a theoretical training. I was so to speak one of the first who had learned theory from scratch.

There were at that time many PhD students and postdocs, who just started to learn theoretical chemistry. The group of theoreticians may have been as large as 20, while the total number of co-workers in Hartmann's institute was about 100. Seen from that aspect the theoretical group still was only a minority, yet I must add it was in high esteem because Hartmann had a great interest in theory.

It was in the beginning 60s when Hartmann had already begun to hold his Summer schools at Konstanz (*Constance lies in Germany, at the Swiss border on Lake Constance – I.n.*) in an old building of an engineering school. Lectures were given to chemists with little knowledge of theoretical chemistry. Essentially it looked like this: there were lectures and exercises for 3 weeks. In 1963 when I started with Hartmann, while I was still working on my masters thesis, I was already helping him. I had to conduct one of these exercises and many people older than I were there. For example I also trained Mr. Bock (14) (Prof. of Inorganic Chemistry at Frankfurt and Munich), even though he probably wouldn't want to hear this any longer nowadays (*laughs*). But of course I did not give the lecture. Bock in those days was Habilitand (e.g. working towards a professorship) one has to add, when I was writing my doctoral thesis. Some years later he has written together with Heilbronner these (15) fairly well known books (16).

**A:** These books are still liked very much by the students.

**J:** Since this was a possibility to include chemistry more extensively. Which was necessary at this time.

**A:** Has Bock actually been working on theoretical problems in these days?

**J:** Bock has never claimed to be a theoretician, at least not in the presence of theoreticians. He is a user, of course he has a great interest in theory and in his Habilitation - he has done a little excursion into something which might be called theory (17). That was in Munich. I am not sure under which auspices Bock had made his work. But anyway, he was participating there in these days as did many others.

**A:** As a physicist you did of course have a mathematical advantage?

**J:** Yes, o yes. Well, I myself participated only three times in these summer schools. The very first, where I was not present, covered ligand field theory. The second was in 1963 and dealt with pi electron systems and Parr (18) was there, of course, but also Fukui (19) was present. But his presentation was only very, very hard to understand since his English was poor. And I did not perceive the implications of his work at that time, mainly because I could not understand his English. Also McWeeny (20) was present, many well-known people.

**A:** Also Mme Pullman? In her interview (21) she told me that she also had been at Constance at some time.

**J:** No, that certainly must have been much later. No, not in the early sixties. Later on there was a summer school every 2 years, and some of which had already taken on the character of a symposium. In 1965 there was one on kinetics in which Hershbach was present, Nikitin and - - -

**A:** Daudel?

**J:** Daudel (24) was not there. I still have all these summer school materials, I could find out who was present then (*laughs*). But then Hartmann started already to think about going beyond the summer schools in the sense that we as theoreticians had to pronounce ourselves more strongly somehow. At that time we were only a handful. Therefore he inaugurated in April of 1965 a Symposium of Theoretical Chemistry which he organized solely himself. The first one took place in Frankfurt for this very reason (25). That was shortly before I was finishing my {doctoral, *I. n.*} thesis (26). I had already finished the work and Hartmann had already referred to it in his presentation - of course I could not present it myself. There were people present like Ruch (27), as well as older ones and who are nearly completely unknown nowadays. Preuß (28), and also Kutzelnigg were already there and a few others. 30 years later I organized the symposium myself, here in the vicinity of Hannover (30). And there were only about 10 people left those who had participated in 1965. Time has apparently passed very quickly if one looks back. And these symposia have had certain effects to enforce certain ideas. There were also the semiempirical ideas, still at the Hueckel level. Hartmann himself was still working on them ...

**A:** May I interrupt you briefly. Very interesting your story; I have been told by someone in a somewhat ironic way that Hartmann "improved" the Hückel theory. Was there a mistake in that improvement?

**J:** It was a paper on the extension of the basis set (31): Well, the 2p orbitals, that has been the normal thing and which were being used in pi systems; so now he wanted to add 3p, in order to prove a rule, the so-called rule of Scheibe (32), which was very much on his mind. But not only he had worked on it, also Ruch had worked on that (33). With this expansion one might have explained that phenomenon in principle yet I would dare to say that the whole thing was abandoned in the end because one would have needed more functions, and also that the 3d would have been more important to add.

**A:** So to talk ironically about that would be exaggerated?

**J:** Yes, I would put it like that: The idea of a development which has been surpassed comes to an end. It has been like this in this case. It was a try which seemed interesting at the time since reflections about an expansion of a basis set are always interesting.

**A:** There were no formal mistakes in it?

**J:** No. But I think except for the symmetry where one should have taken the 3d orbitals instead - no, there were no principal errors in it. But it must be stated that the leap which one did at the time simply wasn't large enough.

**A:** After you had received your doctoral degree - - -

**J:** Later on I was also the head of the editorial office of *Theoretica Chimica Acta* (34) after my thesis. Well, I was 25 years when I - - -

**A:** You did a lot of reviews during that time as well - you have been very diligent!

**J:** Then I was 26 years old. Well those reviews I actually wrote somewhat against the mood of Hartmann. These books were the *Advances in Quantum Chemistry*. Löwdin at the time had handed out the so-called *Green Booklets* (35), for internal usage, which at first were not published but which were used in his Summer Schools. I still have got some of these *Green Booklets*. Hartmann was a little bit sceptical about them. On the other hand these were already one step ahead, a whole series, where one could write *Reviews* about the advances in quantum chemistry. And since the publishing house was also interested in having books reviewed they all arrived at my desk, since I was the editor's chief associate. At that time I did not have much money and these books cost 180 Deutsch Marks (some 50 dollars at that time) and I therefore thought that I save the money of the purchase as well as learning all the things that were covered in there

Well, that was in my own interest. I wrote several *Reviews* and then in 1967, two years after my thesis, I went for a second time to Uppsala to attend the Summer School. Then Löwdin had of course read my reviews and was very pleased with it. He therefore offered me to continue my reviewing which was of course important since these volumes were not so well known in these days. If one sells only a few copies of them, then of course the wide impact is not of any consequence. Well, I think that in this manner many people heard about these *Advances in Quantum Chemistry* (36). There they are still on my book shelf, by the way - but at some stage I stopped to buy them. I have reviewed eight of them. And then I figured, well, enough is enough., maybe someone else should write about them now. In the meantime there are about 20 volumes. In those days that had been a highly interesting matter. I learned quantum chemistry on a broad base.

But mainly there were semiempirical manuscripts submitted to this journal, also by Pullman naturally, and even by Ladik (37), Berthier (38) - certainly, all these papers I have read. Our system was strongly locally oriented at the time. My predecessor, Mr. von Hirschhausen, was the first head of the editorial office, but he worked on his doctoral thesis at the same time. One day Hartmann said: well, he will now have to finish his doctoral thesis. And he offered me, as soon as I would have finished my PhD, a position as lecture associate, that meant wiping out the black board during his lectures, or to direct the journal. Then I decided to assist him with the journal and therefore von Hirschhausen was relieved. I did the work together with three other associates. Two of the former associates responsible for the journal quitted, because they did not want to work under the direction of such a young man - and the other were only about as old as I was or one or two years older. Only Mr. Reinsch was considerably older and collaborated and was later my successor.

**A:** How did it come to the start of *Theoretica Chimica Acta* (39)? How did the business between Hartmann and the Springer Publishers go?

**J:** Yes, that was very simple. We did everything in Frankfurt. We did not only register the manuscripts, we also reviewed all of them.

Then we sent the manuscripts to Springer and we received a small subsidy from Springer, which we could share, by which we could increase our modest salary somewhat. For the publisher it was very favorable.

**A:** Excuse me - has Springer approached Hartmann or vice versa? Do you know how it was?

**J:** I do not know it exactly, because the journal existed already half or three quarters of a year before I became a member of the institute. And when I took charge of the journal, 1965, it was only two and a half years old. But everything went smoothly; the people in charge at the publisher's were a married couple, the Mayer-Kaupps. They were our contact to Springer; I had contact with Mrs. Mayer-Kaupp. I assume that Dr. Mayer-Kaupp was a chemist, if I remember correctly. Later Mr. Boschke came and now there are others. But during the two years of my job as head of the editorial office, I had contact only with Mrs. Mayer-Kaupp mainly by phone, everything went in a very simple way. The only thing that changed during my time there was that I realized that the journal was growing. In the beginning there were few manuscripts. But their number increased more and more and I reviewed again and again and also others - - -

And now I come to the main point: why I got interested in semiempirical methods. On one hand, because a large portion of the manuscript was about such methods, and on the other hand, because Hartmann left everything to us due to his limited time. I see today – at that time I did not quite understand it - how it is, if you have very little time. We asked him only in critical cases – and these I do not want to discuss right now - -. We had to understand semiempirical methods. We knew them in part, but we had to learn more, in order to understand them better and at this occasion I found out that there existed already systematic work by Lykos and Parr from the 50's (40) - - -

**A:** And the book by Parr (41) - - -

**J:** Parr sits even here, there across behind you - (point to his book shelf), I bought it relatively quickly at that time, the other one is the new book by Parr, about DFT (95b). On the contents of his first book Parr lectured already in Constance in '63. Shortly afterwards, in the same year the book was published. I knew Parr from there since '63 and I was naturally interested in these methods. When I decided that I needed a change of location - I had studied in Frankfurt, was there for eight years - I went to Chicago. I had written to several people and the fastest positive response was by Peter Lykos who said that he had money for research. I could not go to Martin Karplus, who was also interested, but had no opening for a postdoc and who referred me to NATO, but they had no stipends at that time (43). I thought, well, I always wanted to learn more about semiempirical methods, so I shall go to Chicago and I learn that.

But the disappointment was quite great: when I arrived, Peter Lykos did no longer work on these methods. Of course it was already 1967, and he started with ab initio methods and wanted to add configuration interaction. Within three months I wrote a special program, about MC-SCF. The first papers were from that time. At the University of Chicago, there was Mr. Hinze (44) already as an Assistant Professor, who wrote more general programs of this kind. I was postdoc at the Illinois Institute of Technology.

The other one who wrote such programs in Argonne was A. C. Wahl (45). And Lykos had this idea that he could also do this. A PhD student of Lykos, who was looked after by Wahl, was writing a special MC-SCF program frame. But at that time he was sitting there for already four years and Lykos thought that the student should finish, because the work was pressing. He gave me this task and I wrote the program in three months, whereabout the student became quite nervous, because I got ahead of him in a short time. The consequence was that Mr. Wahl bluntly cut me off his integral program. We had to climb hand over hand and I had the idea to use the program by McLean and Yoshimine written for small molecules (46). I interfered in the program, took out the integrals. This was also connected with complications ( *pondering l. n.*) - - -. In this way we sailed around the cliffs.

It was a small, but efficient group with Lykos, four, five people, all PhD students, I was the only postdoc. During this time there were seminars held and Lykos had the idea that I should also present a seminar series. I gave 12 seminar lectures in 12 consecutive weeks, that was the whole semester. I had prepared myself by reading the journal literature, this means by Parr, by Pople (47), by Fischer-Hjalmars (48), by Koutecky (49) – and by all those present at the time. Probably I did this quite well so that Lykos proposed that I should put it in writing. I was still very young then and have said to myself: well, I did it all on my own, in consequence I write a manuscript with only my name on it.

This was very, very unusual by American standards, because normally also Lykos' name had to be included. But he did not only tolerate it, but supported me, because he was very

generous, and therefore we are still in friendly contact, although he is 12 years older and is already past his 70<sup>th</sup> birthday. My main achievement was this seminar series on semiempirical methods, the other problem could not be solved, because we did not get access to the integrals for my MC-SCF program (*laughs, l. n.*).

Upon the suggestion of Lykos I made a manuscript out of the material. The longest that I have ever written in my life except of course for my book, it had 80 typewritten pages. I sent it to all well known people in the field, I think also to Berthier and others, altogether I think

to seven people. And all reacted very positively, and it was very difficult to read all these papers. I had put their information in a united nomenclature so that the methods could be compared, I had then put them on different levels. For instance Ruedenberg is also included in this article and clearly Ruedenberg (50) had still a great interest in semiempirical methods at that time. Shortly before, Pople had published this second series CNDO (51), NDDO (52), INDO (53) and he found a compromise with INDO. CNDO was the complete neglect of overlap, NDDO was already a relatively small neglect, it was very difficult to implement it in a short time. These methods did not function very well at first, the accuracy was not high enough and therefore Pople left the field (54). He had put about three years in this development, although he could have achieved further improvements with good coworkers. He himself did not see any possibility to make improvements in a short time and then turned to *ab initio* calculations, to Gaussian functions, which he did not introduce, but Boys (55) and which later in the 60s were worked on by Preuß, (56).

**A:** McWeeny claims that he had Gaussians already before Boys. He did some work on crystallography (57) as a physicist, and there he ran across it, he said in his interview (58). I must have been in the air, perhaps there was a certain parallelism?

**J:** This is quite conceivable, because many of these publications are simply forgotten. I myself have also written a paper about the Hückel method. This was published in the Journal of Chemical Physics, 1969 (59). I have recently read again what the problem was: The Hückel method produces orbital energies which at the same time as a sum result in the total energy, while the SCF procedure, which was interpreted by Fischer-Hjalmars into the Hückel method, does not permit to represent the total energy as sum of orbital energies: This discrepancy can be easily removed if the operator is slightly differently defined. This was still an interesting exercise at that time, which went parallel to my *Review* and which somewhat supported the interpretation by Fischer-Hjalmars. To be sure it was after Pople, his second series of papers (60). But the understanding for the even simpler methods came surely very late, this was done by Fischer-Hjalmars at about 1965 (61). I did not know her personally at that time.

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By the way, I had also written to Hoffmann (62), of course also because he had contributed a lot to the field, to mention this. My contact with Hoffmann dates back to that time when I wrote my *Review* article. Today he is a friend of mine.

**A:** Where is Hoffmann today?

**J:** He is at Cornell, Ithaca, New York. This is a little bit north of New York city. There it is quite nice. I was there only once, 1980, a year before he received the Nobel Prize and he had great quarrels with Dewar (63) at that time.

Dewar was a somewhat curious man, I did not know him personally for a long time. I got to know him only 1976. Hoffmann I had met earlier in 73, that was also in the USA at a conference and Hoffmann was always a great diplomat. He was very decided in his opinion, but which he did not always express in an outright way. Dewar was seeking a controversy already sooner (64).

At the beginning of the 70s I looked around in the USA, sent applications, somewhat naively, you could say: I have simply written to the best universities and I thought that I would receive an answer and then they could see what my capabilities are and that I would perhaps be invited. In general this is not so, the people look around themselves for a candidate and invite him. Among others I sent a letter to Berkeley that I would apply for the position of assistant professor; at that time Pimentel (65) was chairman. He wrote a very nice letter with the following resume: "We acknowledge receipt of your application, many thanks, we will put it on file." This means that they would put it into a folder. But I did not know that much English, that it means that he would probably never look at it again, because there were already so many others in it - and unfortunately that was true.

When I talked also with Lykos about how such an application works, I informed myself about open positions for a theoretician and there was an opening in St. Louis. But it was not precisely for a theoretician. I wrote to the department and the head of appointment committee wrote back: "It is very nice that you have applied. This year we decided for an inorganic chemist, but we want to recruit further university teachers and next year there will probably be another position". I said to myself, okay, it does not matter, I apply again. I simply wrote on the supposition that this is so and I was also invited. And I had to stand up already against young American colleagues. It was not so simple for a German to establish himself - however, I succeeded. Fortunately, also against people who came from Harvard and who would have liked a position in St. Louis. There was even a person, who as theoretician was an assistant professor at the university of Illinois at Urbana, and there was a rumour that he would not receive tenure, he was to be sent to St. Louis. But the people in St. Louis thought, we do not want somebody whom they tried to get rid off, we really want a young man who has great plans.

The expectations were very high in St. Louis - unfortunately there was a recession at the beginning of the 70s, and there was a sudden decline, many left, and the department continuously decreased. But in the beginning, 1969, when I started, I was only 29, I had great luck. I had even younger colleagues, one colleague was only 27. This was quite usual then, when somebody had finished at a good American University, he would work only one year as a postdoc. If one would finish at 25, one could already be an assistant professor at 26. And earlier I was always wondering why such people as Gell-Mann (66), who won the Nobel Prize at 40, was already a world wide leading scientist for 16 years. I found this curious - he was then only 24 - but Gell-Mann was already an associate professor at 24, he would have to have finished at 23 and have made a quick career.

That was of course possible in the USA, but naturally not in Germany. Hopeless. There is this habilitation procedure. I have here an outstanding habilitand who will soon get a position elsewhere, even though not in Germany, he is writing his habilitation thesis for some time. The development of a new method costs years and the writing is very wearisome. I did not go through the habilitation procedure, because I was promoted to the position of associate professor with tenure after two years. And then also the colleagues in Germany said, now he is a genuine professor. And the colleagues whose names I do not want to mention, had written up to that time "Dr. Jug". Well, an assistant professor was not a real professor in the German sense, but there in the USA I had the opportunity to do something on my own. And this is exactly what you have addressed. I had seen that people had stopped working on semiempirical methods. Therefore I thought that this is a good opportunity to improve something. And I started with it, of course (*pondering, l. n.*)

Then a lucky chance helped, at about 1971, when I was already two years in St. Louis and I still did not have a single coworker. Finally, somebody came (*pondering*) at the moment when I was a few months in Germany, in the summer of 1971. In the USA one will formally not receive a salary in the summer, one gets a 9 month contract. Per month the salary is not so bad, but one has to redistribute it over the whole year, in this way one has to save for the three unpaid months. And I thought that it would not be bad if I would work then elsewhere. I have worked as a visiting professor: one time in 1970 at Florida State university in Tallahassee. Originally I wanted to work with Michael Kasha (67), because I was interested in radiationless transitions. Finally, I worked with Rhodes, because Kasha was on leave that summer. Then, 1971, I was visiting professor at Johns Hopkins University with Parr, only one month, then with Labhart (68) in Zürich. This strengthened my contacts and improved my salary.

During this time I had of course already my own ideas, how one could develop semiempirical methods, and when I returned then in 1971 to St. Louis, there came this student, Patrick Coffey. He had already a master's degree in organic chemistry, but he really wanted to do some programming. And this was of course possible only with me. To write a program he had already learned in the army. He wanted to use this skill, and that was not bad for work in theoretical chemistry, Then I said that I had a visiting professorship for one year, which I would start in '72 with Preuß in Stuttgart. Preuß had taken care of it, I knew him already from Frankfurt and the summer school of '63, where he lectured about the LCAO method and I did the exercise session For Preuß who was in 1963 still Privatdozent - -

**A:** Actually he was Privatdozent for a very long time.

**J:** Yes, until 1969, when he went to Stuttgart. He was there for two years and he had applied for my visiting professorship. Thus I was officially visiting professor of the University of Stuttgart and I received a letter not only from Preuß, but also from the president of the University. And there Mr. Coffey came with me, where his task was to develop this semiempirical procedure as PhD thesis (69). What we did was very simple: we said to ourselves, we want to improve the method of Pople. I still teach this in my lecture: His results were really so poor that we could hope to improve them, if we worked on it. I had sufficiently dealt with these formulas already at Lykos' lab and I had noticed that Pople had inadvertently taken a formula from the old Hückel theory, this formula for the resonance integral which in this form had to be wrong. It was simply not tenable, therefore the method failed.

With this little trick, to derive the formula now correctly - - - there was a small paper by Linderberg, who was with Löwdin in Sweden and later Professor in Denmark, about this integral (70). I looked at it, worked myself through it - my first papers were about this integral. And I built this knowledge (70a-b) into the Pople method. I changed it and the PhD candidate became my fasted student up to now, nobody else managed to be that fast. He needed only one and a half years for his PhD thesis and then he had to wait half a year for his PhD certificate. He was already away as a postdoc, after one and a half years already with van Wazer (71). Actually he wanted to work with Dewar and I had tried to get him in contact with Dewar, but Dewar had no opening and he informed me of van Wazer's interest, where the student then stayed. Coffey has developed our semiempirical method as a PhD student (72a-b), but without a name, I assigned it only two years later, because we were not that presumptuous at that time to give our method its own name. This work was published without the name SINDO 1973 in the *Journal of the American Chemical Society* (72a).

When I noticed that one has to give the method a name because it is otherwise not recognized from the outside, I have called our procedure SINDO (73). The procedure interested immediately the referee. I am sure who it was: it was Whitehead, in Canada (74). Whitehead had about 70 parameters and I had perhaps 7, he was very impressed that one could do so much with so few parameters! But in the meantime Dewar had already developed his MINDO method (75) and Dewar was not only much older, more than 20 years, but he had also a huge group of coworkers and he could, of course, work much faster than I could with one or subsequently no coworker.

When I recognized that it would very, very difficult in St. Louis in the course of time - during the year in Stuttgart I could, of course, do a few other calculations with the computer, which were not possible in St. Louis, I had to think about whether I wanted to stay there. To find another position in der USA was too difficult at that time, the situation was too bad in '71, '72, there was an economic recession. Therefore I tried to find a position in Germany. In 1972 I was already invited by several universities, for instance for positions such as the one in Bonn, where Mrs. Peyerimhoff (76) is, then also in Bochum, which today Kutzelnigg occupies and for which I was among the few seriously considered. Now then (*pondering, l. n.*) - one had from the outside still a certain view, beyond Germany. My final success lies also in the fact that I had two referees who obviously wrote always positive things about me. This was Hartmann on one hand and Löwdin (77) on the other hand.

**A:** But Löwdin is no semiempiricist?

**J:** Of course, he worked more methodically, and I would like to say, with respect to Nobel Prizes, Löwdin could have received one. But sometimes the constellation is not so and one is asking why this person and not the other one.

**A:** Well, Löwdin (77) told at the occasion of receiving an honorary doctoral degree from the University of Constance that he himself was a member of the Nobel committee for many years.

**J:** In physics. He was in the physics committee, but that was too close to chemistry. Many tried to nominate him, and I think that there was not a sufficient number, always in the same year. This year's Nobel Prize is of course not by accident -

**A:** Why did they go like that?

**J:** I think you should read the article by Kutzelnigg, which appeared in the *Blaue Blätter* (78), now three days ago (*pondering, l. n.*) – the comments on the Nobel Prizes. Well, - (*pondering, l. n.*). There is large group of people, who can be identified by the comments in the internet. I have it in writing. A colleague has printed it and given it to me (79). I myself had not yet searched for it. At the end there is a little annex and there are also a few references; and from these one can see who is behind it.

**A:** How can one find it? Under Nobel Prize?

**J:** No, this is a little difficult. You have to look for the Academy, in Stockholm. It has an abbreviation. You have to look for the Academy of Sciences, and then you can find it (*laughs*). It is of course so particularly interesting that people has received the Nobel Prize this time, where I stand fully behind it because I know Pople for 30 years. I got to know him about '68 or '69 in Florida. He is not very talkative, if you do not know him. Then I was still very young and I tried to start a conversation, which finished somewhat like this: I asked a question, and he gave a very short answer and then the conversation was finished. In the course of years our conversazions became longer and longer. Now they would be very long, if he had time.

**A:** Please, allow me a change of topic Prof. Jug.

Yesterday evening I could talk with Prof. Tietz, who was Hückel's assistant in Marburg and who became later professor of mathematics in Hannover. Hückel mentions him bei name in his autobiography. The conversation with Prof. Tietz was very instructive (80). In this conversation I was more concerned with the humane aspect of Hückel in Marburg. Unfortunately, for other reasons I could not participate at the celebration of Hückel's 100<sup>th</sup> birthday. His autobiography is not read anywhere. Do you know Hückel's autobiography (81). What do you think about it?

**J:** I it is here on my shelf, of course, I have read it. Hückel is a rare case of a misunderstood scientist. And when you think about that his brother, the chemist was much better known than he was and has written such a big book on organic chemistry (82), and the poor Hückel - I mean - who had two habilitation degrees, who was simply no real physicist and no real chemist. And therefore was not accepted in certain circles. This came only after the war. Of course I have read his papers from the 30s, they were original and pioncering for that time. More intuitive perhaps, but Hückel as a physicist was capable to solve such mathematical problems easily.

The main development came from the physicists, that one has to say – it came from physics. Mulliken (83) and, yes, Heitler (84) in Zürich. I have listened to Heitler's lecture when I was a visiting professor at the University of Zürich, 1971, then Heiter was still lecturing. But there were one five or six student in the audience. Many people know Heitler only by name. But people like Heitler knew a lot of mathematics. And there was a similar situation in Germany. In the first generation of theoretical chemists, there were real chemists among them (*pondering, l. n.*), who had learned only chemistry, and then the physicists came, too. In the second generation there were many physicists. Preuß, Peyerimhoff, too, are from physics, have studied physics. And thus - yes, this possibility to have a command of mathematics was absolutely relevant. And today we are again at this point.

Consequently there is this connection: how can one develop semiempirical methods? By a great deal of mathematics and some sense how it could function. And there semiempirical methods, as I say sometimes, are the least understood methods, because they are actually the most difficult. The improvements are not trivial, you cannot achieve them systematically. You cannot sit down and say, I take an additional function or I take some more correlation, that does not work. And you have to file an internal system, which yields certain things and others obviously not. But the limits have not yet been reached and therefore many of these methods are still valid.

Along the lines of Dewar they were further developed. He started with MINDO, the next he named MINDO/2, with an oblique line, and then MINDO/3. We had once a guest, who of course was not a theoretician, who spoke of MINDO third because of the oblique line (*laughs*) - - - . And these methods were applied also by people, who had no idea about them, who did not even know who to pronounce them - MINDO third, shortly afterwards MNDO came along, I gave a seminar lecture there at Dewar's place, 1976. he had invited me, because I was going to a conference close by, in New Orleans. Thus I had reported about SINDO at that time, that was the oldest version. There was still not a great improvement compared to the one that Coffey had done. But we had already started with interesting

problems, namely thermal reactions. It was about the activation energy of cyclopropane to propene, for example. There was an activation energy of 62 kcal/mol, and I think we had 48 kcal/mol. I talked about that, there were many people, a large audience, and as the host Dewar finally said: "I am sure this is on the mind of many of my coworkers to ask something, but nobody dares to do it, therefore I must do it: Why do you use such a poor method?" (*laughs*). Then I replied: "Yes, Professor Dewar, the reason is this: you have 70 parameters, but I have only 7." But then I became shrewder, and I said to myself: "If I can do it with 14 parameters as well as somebody else with 70, then I am better." I started as a purist in Hartmann's institute, we learned Hartmann methodology.

**A:** Was Hartmann a physicist or chemist?

**J:** He was a chemist, obtained his PhD with Wulff (85), has worked also a few months with Sommerfeld (86), yes, yes, he has really worked with Sommerfeld, that was certainly the highlight of his studies, in the 40s.

**A:** I did not want to interrupt you.

**J:** Yes, Dewar was very direct. And Matsen (87) who was much more involved in formalistic development, told me afterwards: "Alas, Dewar has not seen how beautiful your theory is. It is theoretically so neatly derived, everything is structured." Semiempirical methods still move in this field, they are supposed to be theoretically impeccable, but also very effective. They have to sacrifice a part of the theory for this accuracy. It is like a domino game: something collapses and you have to build everything anew.

**A:** How is it: the ab initio people say, the semiempiricists calculate at zero Kelvin - - -

**J:** This is also no longer true. This year we finished a PhD thesis. Just a month ago Mr. Ahlswede received his PhD degree with the further development of our method, where the heat of formation at room temperature is included (88). Not like Dewar and subsequent papers where the zero-point energy is not included. Mr. Ahlswede included the vibrational energy. He adjusts to achieve agreement with experimental data, but also with ab initio calculations. We can do it, too. We took zero point energies at zero kelvin up to now, but this year at 298 Kelvin. This is also a significant progress. Besides the numerical accuracy is now as good as that of Pople's standard methods, for which he received the Nobel prize. Pople has achieved a great improvement of the GAUSSIAN program and it is, of course, much quoted. But our accuracy is about as good as that of 6-31G\*, for structures.

**A:** With shorter computer times?

**J:** With substantially shorter computer times. But it is absolutely uninteresting for us to treat these small systems, this one can do also ab initio. Certainly at a greater expense, but one can increase the accuracy further and further. Our domain is now the calculation of very large systems, there we are leading.

**A:** The industry maintains that today's semiempirical programs are in part not yet useful. And in industry there seems to be a certain disappointment with respect to quantum chemistry. What is your view?

**J:** Yes, but there is a simple explanation. They have tried to focus on pharmaceuticals. And (*laughs*), these are the chemical systems which are partially quite large. If you grind it through a mill and obtain a structure, then this is of no relevance for the reactivity of such compounds. The procedure is much more complex. By accident we have also worked in this field, because one of my coworkers, who was a biochemistry student by training, wanted to solve a certain problem. We had a cooperation with a biochemist who is now in Cologne, but was before in Brunswick. And we have calculated a system with 8000 atoms - although not with SINDO, still simpler. And to deal computationally with the reactive center, people from industry can not do that, they do not have the means. This is research work for which industry has no time. To take a program and to calculate something very quickly, that does not work. I know that there was somebody at Schering who came from Labhart and worked on such questions. It did not work out the way, one had hoped for. I see better perspectives in the field of adsorption at surfaces, not at all surfaces, at metals it will be very difficult.

**A:** With which program?

**J:** Well, let us say we can treat 1000 atoms with SINDO. This is an appreciable number. Jimmy Stewart sells his PM3 (89). Some time ago he was also with Dewar, but he had some disagreement with Dewar, he works now for Fujitsu (90), but has also his own company Stewart Computational Chemistry and retails the PM3 program. PM3 is a spinoff of MNDO. From MNDO there were three further developments: one by Dewar himself, AM1, Austin Model1 (91), -- - he wanted to give it an identifiable name under all circumstances. Stewart had another philosophy: statistical accuracy, where the whole input is used for parametrization. A year ago I was still against it, but today I do not have such a narrow view any more (*pondering, l. n.*). I can surely imagine that one can have greater success in this way. We have just demonstrated that this idea is not wrong. We have been concerned with adsorption upon the special wishes of our colleagues here in Hannover. Adsorption of small molecules at sodium chloride surfaces is still a relatively simple matter. It is also understandable at MgO which is interesting for catalysis. There we have studied among other things the dissociation of water at defective surfaces. But this means of course many years of work, we work on it already for eight years. For this sort of work SINDO is particularly suitable, which we developed from 1980 onwards. '87, '92 were the next stages (92). We tried several times improvements,

twice we failed, but it costs 10 years to make a real improvement. In his PhD thesis Mr. Ahlswede included small MgO clusters in the parametrization - MgO, (MgO)<sub>2</sub>, (Mg)<sub>3</sub>. They can be calculated *ab initio*. We looked how the bond lengths were *ab initio* and then adjusted the bond lengths in SINDO by parametrization accordingly. It turned out that the results automatically improved. So we were very successful whereas previously these clusters were not treated by anybody, at least not in this way, but under other aspects. There are still larger clusters of this kind, but for other purposes, we did not use them in the parametrization, and there are no measurements. And then one can compare with *ab initio* results on small systems and improve the methods. This has been done by several people already.

But at this time there are, I would say, only five methods in the world which are taken seriously. Which can regularly be used for research and which cover a broad range. In addition there are a few methods which were constructed only for special cases.

The significant methods are:

- 1) First, AM1 by Dewar, which was developed from MNDO. Unfortunately, Dewar's successor, one of his last students is not successful, he does not really move. There is SAM1, but nothing much originated from that one.
- 2) The second is from Stewart, PM3.
- 3) The third is by Thiel (93) who worked at one time with Dewar. He created MNDO/d from MNDO by adding d orbitals as polarization functions and in this way has improved the method. But we have these already for a long time. This is not an idea by Thiel, actually it is one that we had first.
- 4) Zerner, of course, has his ZINDO, for spectra (94).
- 5) Finally, our SINDO

The authors just mentioned are, of course, all good friends of mine, who I meet again and again and we talk about it. Fortunately, it is so that there is no unnecessary competition in this small circle so that one of us is thinking that he is better than the rest. Because this is very, very damaging. Thiel asked me many years ago: "Are you still working on improvements? And I said thoughtlessly: "No". Thereupon he said: "Ah, that's good, then I can work on it, we do not have to duplicate everything." When he had finished, there was no other option for me than to start again. After all his new method was better. In this way - - - it can have a positive effect, if you keep it within limits. Many methods can be traced back to Dewar -

**A:** The DFT methods (95), too? Kohn is there - - -?

**J:** Yes, it sounds curious. Walter Kohn (96) is a physicist, who was already forgotten.

Together with Hohenberg he had derived a theorem that says only that a functional of the density for the ground state exists (97). But from this work you can also gather that you can never explicitly write this functional down. This is not possible. He has only shown that one can fulfill two inequalities in this way. There is only one (functional), not two. Since he did not find this functional and since he was certain that it was not possible to write it down analytically - that means to describe density without orbitals, he had a new idea a year later. Namely he went back to orbitals and he built up the density from orbitals, he derived to so-called Kohn-Sham equations (98), which generate Kohn-Sham orbitals. But these are no Hartree-Fock orbitals! In some respect they are cleverer and can already include correlation.

And then people came along who worked on it more puristically. But with this it did not yet function. Then other people came, like Becke (99) who was still quite young at that time, I think he was in his late thirties, and he proposed a gradient corrected functional. This is somewhat curious, because the kinetic energy is not correctly calculated in the Kohn-Sham equations, it is wrong! This correction is now added to the potential energy and one has to have a correction term for it. Becke was among the first successful ones, another one was Perdew (100). They suggested functionals which increased the accuracy enormously. Then more and more people started to work with it and to develop functionals, to test them. In this way a movement started which grew and grew.

And then Parr came about to include Walter Kohn (*in theoretical chemistry*). I know Walter Kohn only from sight, I have seen him only once or twice. He is now always at conferences on density functional theory, sort of a sign-board, a kind of figure-head. Somebody was needed, since otherwise perhaps nobody would have come close to the Nobel Prize. Walter Kohn was present in 1991 at a conference in Menton (101), I know him from this time. He talked about DFT what was then not considered as particularly striking. But in the next five years the improvement were enormous.

Density functional theory is a semiempirical theory, but which can also be improved, much more easily than the real semiempirical theories. One takes functionals, which are empirically chosen. Once I wrote in one of my papers that there are three stages of semiempiricism (102):

- a) The old stage, Hückel, and Pariser-Parr-Pople, these methods are based on the adjustment of certain integrals, one

does not calculate then, one adjusts them to experimental data.

b) The next stage, better stage is if one generates formulas with flexibility. But not the old ones from Hückel; that does not work, one cannot go with these very far. Therefore - creation of formulas. And this is not different in density functional theory. Only their theory is more general, one can build in more orbitals, much more conveniently, and the results will finally be more accurate. One can treat things which do not work semiempirically.

c) The third stage is consistency of parameters within a row of elements. This excludes arbitrariness.

**A:** But do you continue SINDO?

**J:** We have just recently continued its development and it is now enough, it is more improved with fewer parameters.

**A:** Industry always wants the whole periodic system. How many elements can you treat with SINDO now?

**J:** Yes, well, we can only treat the first three rows. And this should be the end, then in the fourth row relativistic effects arise, and one has to do something about it. We have started, as one of the first groups, to include also transition metals semiempirically, scandium to zinc, that works. But the accuracy is lower. Mr. Ahswede has now finished the first two rows, that means including hydrogen, lithium to fluorine, sodium to chlorine. This is very, very good.

We are still working on (the improvement of) the transition metals, if one tries it in the same way, it is painstaking, the accuracy is not yet so high. The reason is that these systems are more complicated due to their d orbitals. The atoms have a spin and there are different orientations, there we have very close-lying states. All those who investigate spectra have this problem. That is very, very difficult. Zerner has trimmed his procedure completely to transition metal compounds, to make it work. For us this would be subsequent work, whether this works now, too. We have studied spectra only occasionally, we had also a guest from Moscow, who has studied such compounds. But we are interested in the adsorption of oxides of transition metals. Titanium dioxide is a catalyst in its rutile and anatase form, vanadium pentoxide is also a catalyst. But the *ab initio* people are not yet there, they cannot do it. There is the problem. Naturally we have cooperations, very many cooperations and one is with Russians. There is a program for research support. There is a Russian group in Novosibirsk at the Academy of Sciences. That is a very good group there -

**A:** Which name is there first?

**J:** Well, Mrs. Lapina does the experiments. She is perhaps not yet so well known. The better known theoretician is Zhidomirov, he is among the Russian semiempiricists perhaps the best known (103). He came originally from Moscow, but is in Novosibirsk already for a long time. He is also already over 60, thus not a young man any more. And there are also many others. We are interested in experimentalists and try to simulate surfaces according to their experiments, then also reactions on surfaces this will have a great future, since in Hannover there is a center of solid state chemistry. We are lucky that we have collaborated there at the right time, because we have a great deal of experience, and this center shall remain and shall be extended. If we had concerned ourselves with pharmaceuticals, we would have to do now organic chemistry.

The point that stirs *me* today more than previously, is simply how my own work is accepted. Which interest is in this work? When one is young, one sets as a goal the solution and presentation of an interesting problem. In the early days the interest in the practical application was of secondary importance. Then it was about maintaining one's ground among the theoretical chemists, the opinions were also already then quite different, and Pople was not the first who did *ab initio* calculations, quite to the contrary, he joined quite late.

Already in the 60s there was the opinion that you can do everything only *ab initio*. And there was Mr. Wahl who advertised a method which I found very strange, which he called *brute force*.

**A:** Was that the paper by Wahl and Das (104)?

**J:** Quite right. He has done something in this field. He collaborated with this Indian for a year. I never got to know him. And Wahl died already, at young age, with 44, that was long ago. Wahl advertised this track, and there was Clementi (105), and there was Roothaan (106), there were many people who had already done it, the whole Roothaan school. And in Germany, of course, Preuß. And Boys in England (107), and his students like Handy (108) today, they have worked on it. And there were these semiempiricists who were never large by number. At first Pople, then only Dewar and then came Zerner again, and then we came and -

**A:** Thiel?

**J:** Thiel came much later, he is much younger. Also Stewart, who was already earlier in this group, but he has made himself very, very well known only in the last 10 years. He has also worked with Pople, his name is among the authors of the GAUSSIAN program (109). He has now his own program, which really deserves the credit that is given to it. It is very, very efficient and naturally very well known. And exactly Stewart is doing the biochemical calculations, whereas we do not do them.

But all I want to tell you is who reads what one writes? It is not only necessary to defend semiempiricism, but to find interested parties - and what we do finds interest. And for the reason that people want to have certain things, there I must make a selection. For understandable reason I have worked for many years on organic systems, this is easier, because the systems are simpler than inorganic ones. But the result is that the resonance by organic chemists, by the true organic chemists is much smaller, although I put in much more time, also methodically, to develop this. We advanced the development of the concept of bond order to understand how bonds are broken. That of Coulson (110) was obsolete, it could no longer be used. To fit it to *ab initio* calculations, not only semiempirically, biradicals, zwitterions, valence - all that has been advanced by us and entered our semiempirical programs, because we wanted to work with it. The resonance of the true organic chemists was relatively low.

And, of course, if somebody like Schleyer (116) says in a discussion on aromaticity: ". . . these are only semiempirical calculations and therefore they do not have such a great importance. . ." then this is simply a great misunderstanding. For theory is something different, don't you agree. And therefore there are, of course, points of friction, where people want to enforce other developments. Schleyer has placed himself now completely on the *ab initio* side, has never claimed that he is a theoretician, but he calculated very much, has published very many papers, has a great influence, rightfully so because of his original ideas. But the opinion that semiempirical methods can not carry you very far in organic chemistry is absolutely erroneous! We have published now a paper together with Katritzky (117) which proves it. But this was one of my few organic papers in the last few years.

We have left this field, also because these cooperations do not function so well. There somebody comes along - I say that now - and says: "Here we have this problem, could you make a calculation?" And then you sit down and work on it and half a year later you meet again and present the result. The same colleague, an organic chemist, then says: "Alas, we have already progressed, that does not interest us any more." I think that the organic chemists have to sit down on their trousers, if they want to keep the interest of theoreticians alive! You can always get somebody who can run a program and generates data with it. But this is also not always trustworthy. Also the GAUSSIAN program can not be run as a black box. You have to understand how much you can achieve with this or that part. I must say, with physical and inorganic chemists - physical chemists for a long time, inorganic chemists for a few years - these cooperations are much more efficient. Because they do not say after half a year: "Alas, that does not interest me any more."

One can turn this around: I could say: "Look, here I have just calculated this interesting phenomenon, can you measure it?" And then these people say, (*laughs*), organic chemists: "Yes but it is poisonous, I do not like to work with it." With such colleagues you can not cooperate. And that I have not found with inorganic chemists, they can also declare anything as poisonous - I have not doubt that this is not so nice.

But when you work on catalysis, on decontamination of the environment and so - that is also a goal which we have, but naturally only little realized - if you are concerned with CO and NO, and you start to measure - this is also not without risk. But it has to be done. And for instance catalysts in cars which are to remove this NO, that can be simulated today, we can calculate it. Only nobody knows, if this model is now perfect, there are a few people who already calculate such systems. We have also done such calculations, but have not published it yet (1998, *l. n.*), because we are not certain that the mechanism works that way, but there are too few experiments which could clarify this. But there is just a change of mind of other colleagues and also it is quite clear: semiempiricism is still interesting for many things and one can do a few things that one can not do *ab initio*! Density functional methods lie somewhere in between, they can manage somewhat larger systems, are somewhat more efficient than the original *ab initio* methods. With semiempirical methods one can do things that one can not be done in such a way with other methods. The field of interest has simply shifted. And the other thing that one can do, one can cover whole rows of elements - chemistry is a comparative science. If I want to calculate substitution effects and I want to grind 50 systems through the mill, then I can do it in the same way as *ab initio*. Only *ab initio* it may need three months in the worst case, whereas semiempirically it will be through within three days. There is the big difference: in industry they want to know something in three days, where to continue - and not after three months.

**A:** Which types of computers do you use? Parallel computer or

**J:** All types. Originally we worked here internally with PCs, but these PCs were at the same time terminals for the central computer in the computer center (111). And this is a regional computer center for Lower Saxony, which is fortunately located in Hannover, and therefore we have a better contact. We are the greatest users of this computer center. But in the meantime this computer center is too small for us and we had to try for our own computer. The computer center has a vector computer with a large storage capacity, but today there are also workstations with large storage which are hardly slower. The computer center has also a parallel computer as well as a workstation cluster.

I learned today, that means a coworker came to me and said: "The computer center wants to donate their discarded workstations to us, which (*laughs*) were working for the whole university." I said: "of course, we take them, we can still use them." This costs money; if we buy some thing like this, this would be 4 times 10000 or 20000 Deutsch Marks per computer, which we would have to spend. And I think they had four of them, and now still three exist. And the person from the computer center asked: "How many do you want." My coworker: "All three."

**A:** Do you program today in FORTRAN? Vectorized?

**J:** Yes, that is natural - it is a difficult problem. We stayed with FORTRAN, of course with all existing versions. This is no longer FORTRAN II, IV or V, I don't know what it is now - 90 or later. Because it proved practical. Long before one had assembler or machine code to speed up the calculations. This is no longer worth the trouble. The compilers are getting better, and they are also tailored to such things. Our programs here, in particular our SINDO, are test programs for the computer center. They use SINDO to test their compiler. If it runs very slowly, they know that their compiler is not yet so good. Sometimes you have to watch your own programming, now parallel computers are being discussed. Parallel computers have a computer power which is smaller than the sum of their parts. But together they can reduce the running time. If you do it sequentially, the job may run for five months, but with parallel computing it may need only a week. But one has to have a program which is conceptually conceived for this sort of machine.

**A:** Who decides about the parallel run? The program or the steering master?

**J:** I don't think that we do it. I do not think that we parallelize, but the compilers are now more advanced. It was tried earlier, but the compilers were not efficient, one had to do it oneself. And I think that the opinion of our computer center – which has to justify its existence again and again - is that it is not meaningful if everybody parallelizes his own program, because then 100 people have to change their program. This is less efficient than to conceive a compiler which adjusts to such questions. And this was exactly the case with vector computers. Some time ago one wanted to vectorize, then one had to do it in the program. A part can be automatically vectorized, but depending on the quality of the compiler it is better or worse. We have done very little to change the program in this direction of changing needs. What we cannot do is: We cannot maintain so many program versions. There was a EU project - Thiel was a participant, I think also Ahlrichs (112) – parallelization attempts (113). Thiel has a parallelized version (114) of MINDO. We, too, had different versions, a small version for a small computer and another one for a large computer. And then we had a periodic program which ran in a different way.

Then I noticed, (*Laughs*): There is an incredible number of people involved in the maintenance of the single parts. We discard now older versions when the new one is running! We have now again everything and built in flexibility. It is dynamic so that only the needed space is provided. It has not proved useful to extend these version because after the responsible coworkers had left, we were unable to improve the program.

**A:** That was also the reason why quantum chemistry will stick with FORTRAN? Somebody wrote that it takes much effort to rewrite a program in the leading language.

**J:** Yes. As long as compilers are written for FORTRAN, it does not matter.

**A:** This is then the task of computer science?

**J:** Yes, but these people are often not interested in the needs of the users as these would like to have it. Only if they think it is an interesting problem also for computer science. But if the need it very great then you can also find people who put an effort into it.

**A:** Do you have free computer time?

**J:** It is free, but fixed by a quota. And there we do not have such a good standing (*Laughs*) - this quota is democratic: according to the number of coworkers. Earlier, when I had very few coworkers my situation was very, very bad. Today I still have more than 10 coworkers and we can do in this way. But we also watch whether the quota is perhaps not so strictly fixed, we put in a effort to run our programs there. We do our calculations on all clusters, in principle we can also do them in Berlin on a Cray (115). In the times of need we look for new sources. This is very likely done by others colleagues, too. But we were also successful with it. But I have to say now: semiempirical methods do not use that much computer time, significantly less than *ab initio* or density functional methods and therefore we can calculate larger system without going beyond the set limits.

**A:** Yes, these were roughly my questions.

**J:** I have not said too much, I think, about the early times - - -

**A:** I think that the presentation of your personal development and the SINDO method gives a good impression of the development of the second generation of quantum chemistry which at the same time exposes the original semiempirical ideas. Professor Jug, thank you for your detailed presentation.

## ***References and Notes***

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At that time very well known by his book *Theorie der chemischen Bindung (2b)*.

**(2b)** H. Hartmann, *Theorie der chemischen Bindung*. Springer, Berlin, 1954.

**(3)** H. Greiner. Professor of Theoretical Physics at the University of Frankfurt.

Author of a long series of textbooks on theoretical physics: volumes 1-10, 1975 -.

**(4)** On the Ising model see textbooks of theoretical physics, e.g. W. Nolting, *Grundkurs Theoretische Physik. Bd. 6: Statistical Physics*. Verlag Zimmermann-Neufang, Ulmen, 1994.

**(5)** C.J. Ballhausen, *Introduction to Ligand Field Theory*. McGraw-Hill, New York, 1962.

**(6)** The computers of Zuse were built from 1936-1964 in Germany.

The first types were electromechanical, the later ones bases on tubes.

**(7)** Three-dimensional box model with step in polar coordinates, in contrast to Kuhn with electronic interaction as perturbation term

**(8)** Quantenchemisches Modell für einen oktaedrischen Titankomplex, Frankfurt 1964.

**(9)** That was about the time of the IBM 704-709 (1955-1958) and the IBM 7080 (1960), respectively.

**(10)** FORTRAN, ALGOL: In the category of algorithmic languages ALGOL and FORTRAN were the first representatives.

FORTRAN came in 1957, ALGOL 1958. FORTRAN IV, appeared first in 1966 was subsequently in use for a long time, since

one could perform almost all calculations in natural sciences. Subroutines, later known as procedure were possible in

FORTRAN for the first time, whereas they were implemented in ALGOL from the beginning. FORTRAN IV did not yet contain

graphical programs, graphical presentations, e. g. for the electronic density of orbitals were partially realized by multiple printed letters.

**(11)** The IBM 7090 came on the market in 1959. It was the first fully transistorized computer. 1962 and 1964 the IBM 7094 and 7094 II appeared.

(12) FORTAN V appeared in 1967.

(13) S. Fraga, Prof. of Theoretical Chemistry, University of Alberta, 1962-1995; now Prof. emerit.

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(15) E. Heilbronner, Prof. of Theoretical Organic Chemistry at the University of Zurich

and later Basel. Together with Bock Author of the books of ref. 16.

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Naturwiss. Fakultät, Ludwig-Maximilians-Universität, München, 1964.

(18) R.G.Parr, born 1922, Prof. of Theoretical Chemistry, Univ of North Carolina, Chapel Hill, USA.

(19) K. Fukui, 1918-1998. Frontier Orbital Theory. Nobel Prize 1981, together with R. Hoffmann. Japanese theoretical chemist with primary interest in chemical reactivity .

(20) R. McWeeny, born 1924, Ph.D. at Oxford under Coulson in 1948. Prof at the Universities Newcastle upon Tyne, Keele and Sheffield. Since 1981 Professor of Theoretical Chemistry at the University of Pisa (being the brother in law of G. Del Re).

See also my interview with R. McWeeny at Pisa 1993.

(21) A. Pullman and B. Pullman. Institut de Biologie Physico-Chimique, Paris.

See also my interview with Mme A. Pullman in Paris in 1997.

(22) D. Herschbach, Prof. of Physical Chemistry. Harvard University. Nobel Prize 1986.

(23) E.E. Nikitin, Russian Academy of Sciences, Moscow, now Technion, Haifa.

(24) R. Daudel. Prof. in Paris.

See also my interview with R. Daudel in Paris in 1997.

(25) Symposium für Theoretische Chemie, Frankfurt 1965.

(26) K. Jug, *Anwendung einer Einzentrenmethode auf die  $\pi$ -Elektronensysteme von Fünferheterocyclen.* Dissertation, Frankfurt 1965.

(27) Ruch, Prof. emerit. at the FU Berlin.

**(28)** H. Preuß, Prof. emerit. of Theoretical Chemistry, University of Stuttgart.

**(29)** W. Kutzelnigg, Prof. of Theoretical Chemistry at the University of Bochum.

See also my interview with W. Kutzelnigg at Bochum in 1997.

**(30)** 31. Symposium on Theoretical Chemistry, Loccum 1995.

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**(35)** Reports of the Quantum Chemistry Group, Uppsala.

**(36)** The *Advances in Quantum Chemistry* were started in 1964.

**(37a)** Janos Ladik, born 1929 in Hungary. Studied chemical engineering in Budapest, thereafter research group leader at the central research Institute for Chemistry at the Hungary Academy of Sciences. 1972 changed to TU Munich as Prof. of Theoretical Chemistry, 1975 call to Erlangen, where he worked as Professor of Theoretical Chemistry until his retirement.

(Quelle: *Erlanger Nachrichten* vom 2.6.1989).

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(47b) J.A. Pople and D.L. Beveridge, *Approximate Molecular Orbital Theory*. McGraw-Hill, New York, 1970.

(48) Inga Fischer-Hjalmars, born 1918 in Stockholm. Later Prof. in Theoretical Physics at the University of Stockholm.

See also my interview with I. Fischer-Hjalmars in Stockholm in 1999.

(49) J. Koutecky. Prof. emerit, FU Berlin.

(50) K. Ruedenberg, born 1920, M.S. in Chemistry and Mathematics, 1944, University of Fribourg, Switzerland, Ph.D. in Theoretical Physics, 1950, University of Zurich, Switzerland.

Associate and Associate Professor of Chemistry and Physics, 1955-62, Iowa State University,

Professor of Chemistry and Physics, 1964-1991, Iowa State University.

Honorary Ph.D.'s from Basel, Bielefeld, Siegen. Editor in Chief of *Theoretica Chimica Acta*

1985-1996, Associate or Advising Editor of many other journals in this field.

(51) CNDO : J. A. Pople D.P. Santry and G.A. Segal, J. Chem. Phys. **43**, S129 (1965).

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Developed the Extended Hückel Method. Together with Woodward 1965 papers on the connection between molecular symmetry and organic reactions. Then came the conservation of orbital symmetry. Nobelprize 1981, together with Fukui.

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(64) P.-O. Löwdin, priv. communication (at my interview with him in June 1999).

(65) G.C. Pimentel, 1922-1990. Prof. of Physical Chemistry, University of California, Berkeley.

(66) Gell-Mann, born 1929, Nobel prize 1969. American physicist, professor at the California

Institute of Technology in Pasadena till 1993.

(67) M. Kasha, Prof. of Chemistry, Florida State University.

(68) H. Labhart, Prof. in Zürich, main time of work at the end of the `60s.

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**(71)** J. von Wazer, Prof. Emeritus of Inorganic Chemistry, Vanderbilt University.

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**(76)** S. Peyerimhoff, Prof. der Theoretical Chemistry, University of Bonn.

**(77)** Per-Olov Löwdin, 1916-2000. Born in Uppsala, Sweden. Ph.D. in Physics 1948. From 1960-1983 professor at the University of Uppsala, in parallel professor at Gainesville, Florida until 1993. He was a member of the Swedish Nobel Committee in Physics for many years. He was the founder of the *International Journal of Quantum Chemistry* and of the series *Advances in Quantum Chemistry*. He started the very famous summer schools of Quantum Chemistry around 1958. In 1955 he came out with what is now known as *Löwdin Orthogonalisation*. In 1998 he obtained a honorary doctor's degree at the University of Constance, one among of many others.

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**(81a)** E. Hückel, 1896 - 1980 Prof. at the University of Marburg (Germany).

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Reprint by Dover Publications, New York, 1984.

**(84b)** W. Heitler, E. London, *Wechselwirkung ....*

Zeitschr. Physik **44**, 455-472 (1927) - one of the classic papers!

**(85)** P. Wulff, 1897-1947. In the considered time period Privatdozent at the University of Frankfurt.

**(86)** A. Sommerfeld, 1868 - 1999. Professor in Clausthal, Aachen and Munich. 1915 Finestructure of the hydrogen spectrum,

1916 Quantum theory of the normal Zeeman effect. Famous through his work and the resulting volumes *Atombau und*

*Spektrallinien*, which can even today convey the foundations of the theory.

**(87)** F.A. Matsen. Published a series of group theoretical papers in chemistry. Left the field to concentrate exclusively on group theory.

**(88-a)** B. Ahlswede, *Quantenchemische Adsorption von Wassermolekülen an defekten NaCl (100)- und MgO (100)-*

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**(93)** W. Thiel, Prof. at the Max-Planck-Institut für Kohlenforschung, Mülheim/Ruhr.

**(94)** M. Zerner 1940-2000. Prof. of Theoretical Chemistry, University of Florida.

**(95)** DFT: Density Functional Theory. See the following three books:

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**(95d)** J.K. Labanowski and J.W. Andzelm (Eds.), *Density Functional Methods in Chemistry*. Springer, New York, 1991.

**(96)** Walter Kohn, born 1923 in Vienna, Austria. 1945 B.A. in Mathematics and Physics at University of Toronto, Toronto, Canada, 1946 M.A. in Applied Mathematics, 1948 Ph.D. in Physics at Harvard University, Cambridge, MA, USA. Prof at the Carnegie Institute of Technology, Pittsburgh, USA from 1950-1960, then Prof. at the University of California, San Diego, USA 1960-1979, followed from the University of California, Santa, Barbara, USA until 1984.

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**(99)** A. Becke, born 1953. Prof of Theoretical Chemistry, Queen's University, Canada.

**(100)** J.P. Perdew, Prof. of Physics, Tulane University.

**(101)** Menton, City in Southern France, at the Riviera, between Monte Carlo and the Italian border.

R. Daudel started the series there together with Pullman in 1973.

**(102)** K. Jug and M. Krack, *Consistent Parametrization of Semiempirical MO Methods*. Int. J. Quantum Chem. **44**, 517 (1992).

**(103a)** G. Zhidomirov, Prof. At the Borekov Institute of Catalysis, Novosibirsk, GUS.

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**(106a)** C.C.J. Roothaan summarized the result of the Mulliken group in his famous paper *(106b)*.

**(106b)** C.C.J. Roothaan, *New Developments in Molecular Orbital Theory*. Rev. Mod. Phys. **23**, 69-89 (1951).

**(107)** S.F. Boys, formerly Reader of Theoretical Chemistry, Cambridge University, UK.

**(108)** N. Handy, Prof. of Theoretical Chemistry, Cambridge University, UK.

**(109)** Gaussians: See books of introductory quantum chemistry. e.g.W. Kutzelnigg, *Einführung in die Theoretische Chemie*. VCH, Weinheim, 1994. p. 526 ff.

**(110a)** C.A. Coulson, 1910-1974, English theoretical chemist who developed a molecular orbital theory and the concept of partial valency. He developed many mathematical techniques for solving chemical and physical problems.

Coulson was born in Dudley, Yorkshire, and studied at Cambridge. He became professor of theoretical physics at King's College, London, 1947, professor of mathematics at Oxford 1952, and later Oxford's first professor of theoretical chemistry. He was chair of the charity Oxfam 1965-71. The molecular orbital theory that Coulson developed is an extension of atomic quantum theory and deals with 'allowed' states of electrons in association with two or more atomic nuclei, treating a molecule as a whole. He was thus able to explain properly phenomena such as the structure of benzene and other conjugated systems, and invoked what he called partial valency to account for the bonding in such compounds as diborane. Coulson also contributed significantly to the understanding of the solid state (particularly metals), such as the structure of graphite and its 'compounds'. He wrote three best-selling books: Waves 1941, Electricity 1948, and Valence 1952. (Taken from the Internet in 4/2001, Source unknown.)

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p. 171 (with respect to Hückel calculations): "Someone said that if you ask me a question before dinner

*I am an optimist - after dinner, I am a pessimist."*

**(111)** The computer center in Hannover became suddenly known to the general public by its excellent search machine *MetaGer*.

**(112)** R. Ahlrichs, Prof. of Theoretical Chemistry, Karlsruhe.

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**(116)** P. von R. Schleyer, Prof. emerit. University of Erlangen, now University of Georgia, USA.

**(117)** A.R. Katritzky, M. Karelson, S. Sild, T.M. Krygowski, K. Jug, *Aromaticity as a Quantitative Concept. Part VII: Aromaticity Reaffirmed as a Multi-Dimensional Characteristic*. *J. Org. Chem.* 63, 5228-5231 (1998).

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