Theor Chem Acc (2010) 126:99–108
DOI 10.1007/s00214-009-0718-6

Jean-Pierre Daudey, a scientific itinerary

The following text, written by a number of close collaborators of Jean-Pierre Daudey, is an attempt to give to the reader a brief overview of the main scientific interests of this outstanding scientist. Of course, due to its very nature, such a text is necessarily partial and sometimes biased towards some scientific aspects. In particular, we are convinced that a number of important collaborators of Jean-Pierre have been forgotten despite our effort of completeness. In advance, we would like to apologize for that.

Jean-Pierre Daudey was born in 1945 in a rural zone on the east of France, in the Jura region. His father was an elementary-school teacher, who transmitted him the virtues of effort and moral behavior of the peasant background, and in his classroom the taste of understanding and reading. He started his superior studies in Lyon and entered the famous and selective *Ecole Polytechnique* in Paris in 1965. Most of the students of this school make successful and wealthy careers in the industry, the banking or in high-ranked government positions, but he chose to pursue a career in science. In 1968 he joined the Laboratory of Professor Bernard Pullman and Doctor Alberte Pullman in the *Institut de Biologie Physico-Chimique*, founded by Edmond de Rotschild, in the heart of the Latin Quarter in Paris. He was attracted by the idea that Quantum Chemistry could build a bridge between Physics and Biology, an idea which was strongly promoted by these two leading personalities, and which receives nowadays the support of powerful and efficient computational tools, at the time not accessible. The years of his Ph.D. work were also a turning point in the practice of Quantum Chemistry. The privilege of π-electron model Hamiltonians and of the special attention to conjugated systems had been abandoned some years before, when the semiempirical treatments of all valence electrons (CNDO type methods) had become popular. But at this time ab initio calculations started to be accessible for polyatomic molecules, at least at the mean-field level. In this laboratory, benefiting from intense discussions with a group of three young enthusiast scientists, Pierre Claverie, Simon Diner and Jean-Paul Malrieu, he touched to the development of rather new codes, such as the semi-empirical PCILO technique, and the first multi-reference ab initio perturbative method, CIPSI. Since he had received in the *Ecole Polytechnique* a good formation in Mathematics and Physics, Alberte Pullman, who directed his Ph.D. (Thèse d'Etat, defended in 1975) engaged him in the calculation of rather complex properties, such as Zero-Field Splitting and NMR shielding tensors. At this time he also exploited an iterative perturbative fulfilment of the Brillouin's theorem, which produces self-consistent non canonical Molecular Orbitals, for instance, localized SCF MOs. A lot of his life-long interests already appear in the papers he published during these years of formation, ranging from technicalities (which are crucial in our discipline) for instance, numerical integration, conceptual

methodology, chemical reactivity and spectroscopy. It may be interesting to mention, for the new generations, that at that time the CNRS offered permanent positions to young scientists, who performed their Ph.D. work with a firm security and much freedom.

Motivated by his social concern and his cultural curiosity he entered in contact with the hispano-american world. He first participated in a summer school in La Habana in 1970 and played a crucial role in a workshop in México City in 1974, around the PCILO program. His deep love for this second country started there and made him choose an unconventional Postdoctoral stay. He spent 2 years (1976–1978) at the Universidad Nacional Autónoma de México (in México City) where he established strong intellectual and friendly interactions with a lot of scientists, among whom Carlos Bunge, Iván Ortega, Manuel Berrondo, and Octavio Novaro. He fluently spoke Spanish and was excellently integrated in this environment, for instance, playing soccer with a suburb team. He loved visiting the various regions of this vast country which gave him a very large knowledge of the historic and sociologic landscape of México. But he had to return to France and decided to join the very small group of the *Laboratoire de Physique Quantique* in Toulouse, created by Philippe Durand in 1969, which had already hosted J.P. Malrieu, coming from the same Parisian lab, in 1974. He brought there a lot of new abilities in this small team, which has grown and is nowadays the largest one in France, a growth which is largely due to the presence and activity of Jean-Pierre. He was technically very efficient, curious, enthusiastic and friendly, creating an excellent atmosphere for the new members of the team, the students and the numerous foreigners, coming for a short stay or a full postdoctoral stay. The fluxes were especially intense with Italy and Spain, and have created durable links.

He was the director of number of Ph.D. theses and his scientific investments cover a very broad range of domains. Looking at the collection of his publications (about 120 papers), it appears that he had a special interest in theoretical spectroscopy, especially the accurate determination of potential energy curves of complex molecular systems. About 60% of his papers are related to this aspect. Since the required accuracy is only accessible through the use of rigorous tools, he was extremely concerned by the methodology and he invested much effort into methodological developments. We may quote his contributions to the treatments of the Many-Body problem, especially in Configuration Interaction algorithms, the three-class CIPSI algorithm in 1983 (with nearly 300 citations), the self-consistent corrections to CI ($(SC)^2CI$) in 1993 (quoted 112 times), later (in 1994) extended to a Multi-Reference version and the Difference-Dedicated CI in 1992 (122 citations) One of his most quoted papers (with J.P. Malrieu and Ph. Durand) introduced the new concept of intermediate effective Hamiltonians, which represents a significant enlargement of the theory of effective Hamiltonians, and has seen broad applications (247 citations).

Another methodological investment concerns the use and development of pseudopotentials (or effective potentials). It starts in 1977 with Alberte Pullman, continues during his stay in México with Berrondo, Novaro and Ortega, and goes on with the creation of core-valence correlation pseudopotential in 1982 (117 citations), later on reformulated with Michel Pélissier. At this time (1988) he proposed a revolutionary specific gaussian basis scheme for such core pseudopotentials (173 citations). This idea, besides diminishing the number of electrons to be treated explicitly, leads to the fact that the pseudopotential monoelectronic integrals can very efficiently be calculated as overlaps, therefore significantly reducing the computational effort. In the same direction Daudey, F. Alary and R. Poteau have worked in the last decade on the concept of chemical-group pseudopotentials. This seducing idea has only partly reached its full potentialities, due to the complexity of the effects that need to be taken into account (electrostatic, steric, electronic delocalization, polarizability, directionality, etc.) and it may be considered that the progress of DFT codes reduce its interest. However, chemists synthesize very complex and large systems these days, and such molecular pseudopotentials can be useful in order to extend the domain of applications of quantum chemistry methods, including DFT. Such methodological developments also originate from the will of Jean-Pierre Daudey to establish a fruitful scientific interaction with experimentalists and to be able to take into account the effect of functional groups as accurately as possible.

These methodological improvements were directed to spectroscopy. For instance, the core-valence correlation potentials enabled him to perform a series of very accurate calculations on alkali diatoms. He also devoted a lot of efforts on the complex spectroscopy of transition metal molecules, in particular, copper and silver halides. In the recent years he was pursuing, with A. Ramírez-Solís and others, a hard fight with the linear triatomic molecules $CuCl_2$ and $AgCl_2$, whose lower electronic spectra are nearly degenerate. They employed all types of methods from quantum Monte Carlo to TDDFT, including nearly size-consistent CI approaches and spin–orbit effects to assess the low-energy transitions of this molecule. These benchmark studies showed two important things: that the accurate transition energies from DFT-based methods can actually arise from spurious error compensations in the exchange–correlation energy of both electronic states, and that the spectroscopy of some small metallic molecules remains an open challenge even for today's most sophisticated quantum chemical methods.

Along with M. Caffarel, J.L. Heully and A. Ramírez-Solís, in 2005 he showed, for the first time, that the most refined version of quantum Monte Carlo approach (fixed-node diffusion quantum Monte Carlo) can now yield accurate enough results to account for the electronic excitations in transition metal atoms, in that instance, for the lower spectrum of the copper atom and its cation.

He was especially successful when he entered the domain of magnetism, another problem involving near-degeneracy, but now between spin multiplets belonging to the same space configuration. The ab initio calculation of the singlet–triplet energy gap in the copper-diacetate dimer seemed an impossible task when the experimentalists of the *Laboratoire de Chimie de Coordination* came to their neighbor theoreticians in search of a computational tool. In 1981 Daudey and Malrieu suggested to calculate directly the energy difference in a perturbative mode, and obtained both a quantitative agreement with experiment and a first tool for the analysis of the physical effects governing the magnitude of the magnetic coupling between the metallic ions. Olivier Kahn gave a large publicity among experimentalists to this work, quoted now over 200 times. Daudey exploited during a few years this method in collaboration with experimentalists, but left the domain, which has benefited later on from other (variational and more accurate) approaches.

In the early 2000s, in addition to his interest for molecular-group pseudopotentials, he had seminal discussions with Odile Eisenstein about chemical complexity. They bemoaned that the dynamics of molecular and extended systems were at that time rarely taken into account by quantum chemists, although it had been considered for a long time in the context of force-field methods and by simulations in condensed matter physics. He then suggested to F. Jolibois, L. Maron and Ch. Raynaud, to develop efficient 'on the fly' ab initio molecular dynamics within standard quantum chemistry codes (i.e. to tackle the problem of developing such methods in localized atomic orbitals basis sets). Then, they successfully studied chemical reactions as well as spectroscopic properties and showed in test cases the importance of dynamical effects.

Jean-Pierre Daudey loved to tackle new problems and to explore new techniques. He was glad to answer positively to the demands of experimentalists. He thought that theoreticians had to try to help in the treatment of radioactive materials and developed theoretical efforts to implement, at a reasonable price, both relativistic corrections and specific calculations on lanthanides and heavy atom-containing molecules. He played an important role both at the French level in collaboration with the French Atomic Energy Commission, and in the construction and scientific animation of a European network devoted to relativistic effects and heavy elements (REHE) which is still very active. Although he had invested so much in the explicit treatment of electron correlation (now called wave function-based methods) he was very interested in the developments of DFT (see a paper of 2000, published with M. Casida et al., 102 citations) and gave numerous lectures on this topic.

He moved on but remained constant in his early interests. He had received an excellent culture on intermolecular forces in his contact with an outstanding scientist, Pierre Claverie, who died in his early forties. One of his early papers (1978) concerns solvent effects and was cited 170 times. He worked on intermolecular forces with O. Novaro, M. Berrondo and W. Kolos, and more recently on cation–water interactions with I. Ortega and A. Ramírez-Solís. He delved into astrochemistry with A. Klotz, to cluster science and solid state physics. His background was essentially that of a physicist, but he could take pleasure in molecular design. In this direction one may quote, for instance, a 1981 work on nitrogen- and phosphorus-based tetrahedral and cubic structures, with G. Trinquier (112 citations), and the collaborations he was starting with the very creative coordination chemistry group of Bruno Chaudret and his collaborators. Fascinated by the possibilities offered by these new materials and wishing to get free of the old structure he had contributed so much to build, he decided, in 2005, to create a new laboratory closely linking experimentalists and theoreticians in Toulouse.

The number of his scientific publications is moderate, but their relevance is attested now by 4300 overall citations; one-third of his articles has been quoted more than 40 times, while 12 of his papers have more than 100 citations. In these days of proliferation of publications this ratio deserves to be mentioned. It is also important to mention his sense of collective responsibility. He never refused the administrative charges which he was asked to exert in the direction of his group/Institute and in the scientific evaluation of external groups or scientists. In 1990 he became head of the *Laboratoire of Physique Quantique* in Toulouse University, a position he kept for more than 8 years. About the same time and around this laboratory, the French scientific institutions decided to create a new Institute, labeled *Institut de Rechercher sur les Systèmes Atomiques et Moléculaires Complexes* and, where specialists of experimental atomic and molecular physics, cluster science, statistical physics and heavy-fermions solid state theory work in good intelligence and interact. J.P. Daudey was the motor driving the creation of this Institute, became its first Director and crucially contributed to its strengthening. But it is perhaps more important and fair to finish this short description of a scientific trajectory evoking his warm personality and his human qualities. He had a broad culture beyond science, he was a great novel

reader (he particularly enjoyed García-Márquez, Vargas-Llosa and Philip Roth), knew Jazz and its musicians very well, curious of social sciences, loved to travel, to hike the Pyrenees, to play soccer and squash, to party and dancing. After 1992, his long-lasting relation with I. Ortega and A. Ramírez-Solís brought him back to México on a yearly basis for well over a decade, so he became rather knowledgeable about Mexican archeology, food, indigenous traditions and Mexican symphonic music.

Some of us were lucky to have him as a caring and committed friend but, for everybody else he always had a smile and the time to try to help in any way he could. Unfortunately, his health and general state deteriorated leading him to leave us prematurely in the fall 2008, after a slow and painful descent, which, to some extent, replicated the theme of one of his favorite novels, Below the Volcano, which he cherished from his twenties.

Quantum chemistry lost a great scientist but we will always remember him as a very special friend, generous and full of human qualities.

Michel Caffarel
Jean-Paul Malrieu
Romuald Poteau
Alejandro Ramírez-Solís

List of publications

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