hc

Doctor Honoris Causa

Evert Jan Baerends

Sovan Lek

Universitat de Girona

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Parlaments de la cerimònia d'investidura llegits
el dia 9 de maig de 2019 a l'Aula Magna de la Facultat de Ciències

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«El Consell de Govern, en sessió ordinària número 4/2017, de 25 de maig de 2017, va adoptar per unanimitat l'acord que, transcrit literalment, diu: **Concessió del títol de Doctor Honoris Causa de la Universitat de Girona al doctor Evert Jan Baerends**, d'acord amb la proposta presentada pel Departament de Química. **Concessió del títol de Doctor Honoris Causa de la Universitat de Girona al doctor Sovan Lek**, d'acord amb la proposta presentada pel Departament de Ciències Ambientals.»


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Investidura Doctor honoris causa
Evert Jan Baerends
Sovan Lek
Universitat de Girona
Facultat de Ciències

Presentació del Dr. Evert Jan Baerends a càrrec del professor Miquel Solà


Dr. Evert Jan Baerends

Introducció

Rector Magnífic de la Universitat de Girona;

presidenta del Consell Social de la Universitat de Girona;

secretari general;

excel·lentíssimes autoritats acadèmiques, polítiques i civils;

prof. Dr. Sovan Lek;

prof. Dr. Emili Garcia-Berthou;

membres de la comunitat universitària;

amigues i amics,

És per a mi un honor presentar avui, juntament amb el Prof. Marcel Swart, en aquesta solemne sessió d'investidura, els mèrits que reuneix el Prof. Evert Jan Baerends per ser investit doctor honoris causa de la nostra universitat.

Aquesta concessió, promoguda pel Departament de Química i amb l'adhesió de l'Institut de Química Computacional i Catàlisi, s'ha fet prenent en consideració els criteris que estableix la normativa de la nostra universitat i, molt especialment, els que es refereixen a les aportacions científiques i a la vinculació del nou doctor honoris causa amb la nostra universitat.

Per qüestions de salut, el Prof. Evert Jan Baerends no ens pot acompanyar avui en aquest acte. Des d'aquí li desitgem una ràpida i total recuperació. Amb el Prof. Marcel Swart hem preparat aquesta presentació dels mèrits del Prof. Evert Jan Baerends i hem decidit que un servidor llegirà aquesta *laudatio* i que el Prof. Marcel Swart llegirà el discurs d'acceptació que ha escrit el Prof. Evert Jan Baerends per a aquesta ocasió.

En la primera part de la presentació ens referirem a les principals aportacions científiques de l'homenatjat i ho farem en anglès per tal que el Prof. Evert Jan Baerends ens pugui seguir. En la segona part comentarem la vinculació del Prof. Evert Jan Baerends amb la Universitat de Girona, i en aquest moment tornarem al català.

Scientific merits

Summarizing the scientific career of Professor Baerends in few words is a very complex task, since his main contribution, beyond his tangible achievements, is his capacity to transmit to collaborators his enthusiasm for discovery and his continued commitment to rigor and truth. Evert Jan Baerends has dedicated his life to science and has spent his career acquiring scientific knowledge and disseminating it to new generations with a passion that is simply an extension of his passion for life in all its facets.

Evert Jan Baerends is professor emeritus of the Vrije Universiteit Amsterdam. He is currently one of the most prominent researchers in the field of theoretical and computational chemistry. He was born in 1945 in Voorst, Friesland, a region of the Netherlands with its own language, like Catalonia. He did his PhD at the Vrije Universiteit Amsterdam under the supervision of Prof. Pieter Ros. During that time, he had to deal with transition-metal complexes. He began to use traditional computational techniques to study these complexes with the Hartree-Fock method, but he soon realized that the results obtained were not reliable. At this time, crystals containing metals were typically studied by physicists using the X_α method, a method based on the density functional theory (DFT). Therefore, he decided to investigate whether methods based on the DFT were feasible in transition metal chemistry. It was a brave, somewhat quixotic quest (for a man who, incidentally, physically resembles the Quixote). No one had used the DFT method in chemistry before, so he had to program his own code to perform the simulations. He adopted pragmatic and efficient numerical approaches to generate his own Hartree-Fock-Slater (HFS) program, which later became the Amsterdam Molecule (AMOL) code currently used by many computational chemists as the Amsterdam Density Functional (ADF) program. The program stands out for its unique features such as Slater orbitals and the pioneering use of precise numerical integration, density fitting, linear scaling, and parallelization techniques. Since the 1970s, Prof. Baerends and his collaborators, with special mention of the late Prof. Tom Ziegler, have demonstrated the utility of DFT tools for computational chemistry studies. Twenty years after the first DFT calculations by Baerends, the 1992 release of the Gaussian program incorporated the DFT methods. As a result, DFT methods became highly popular in the theoretical and computational chemistry community. In 1998 the Nobel Prize in Chemistry was awarded to Walter Kohn "for his development of the density-functional theory" and to John A. Pople "for his development of computational methods in quantum chemistry." Today DFT has become the computational quantum mechanical modelling method most used in physics, chemistry, and material science to investigate the electronic structure of atoms, molecules, and condensed phases. The DFT method reached this level of popularity thanks to the work of Prof. Baerends and collaborators who proved its utility. Many of us consider it unfair to have excluded Prof. Baerends from the list of awardees of the 1998 Nobel Prize in Chemistry.

Now I will briefly refer to other relevant works of Evert Jan Baerends. He complemented the aforementioned ADF program with the BAND DFT program, which extended the molecular treatment to periodic systems. Also in this field, Prof. Baerends has made significant contributions. He elucidated the connection between properties of the exchange-correlation (xc) potential and that of the so-called exchange-correlation hole. In this way, he was able to improve the calculation of response properties and time-dependent DFT. He has also explored the relationship between the density matrix and the xc-hole. In later studies, he developed density matrix functionals, the basis of the density matrix functional theory, opening up a promising avenue to improve current DFT methods. He analyzed chemical bonding and chemical interactions, a central aspect of chemistry, using Morokuma's energy decomposition analysis as implemented in ADF, and mastered the treatment of relativistic effects on electronic structure. He developed the efficient and widely used zeroth-order regular approximation (ZORA), which is very well suited for application with density functional theory. Finally, the Baerends group also developed a multilevel approach entirely based on DFT. In particular, he used a frozen-density embedding (FDE) method to calculate properties, such as UV-Vis spectra, electron paramagnetic resonance hyperfine coupling constants, and circular dichroism spectra, of molecules in solvents.

He has made these important scientific contributions in more than 450 papers that have received more than 50000 citations. His h index is 98. Among his many other distinctions, let us mention the prestigious Schrödinger Medal of the World Association of Theoretical and Computational Chemists (WATOC), which he was awarded in 2010 for his pioneering contributions to the development of computational density functional methods and his fundamental contributions to density functional theory and density matrix theory.

Relacions amb la UdG

El Prof. Baerends ha col·laborat amb molts dels químics teòrics més prestigiosos del món. Però per a nosaltres és un orgull poder destacar que el Prof. Baerends ha inspirat la recerca i ha contribuït decisivament a la formació i consolidació de moltes persones que actualment formen part del Departament de Química i de l'Institut de Química Computacional i Catàlisi (IQCC). La col·laboració que es va iniciar fa vint-i-cinc anys, quan vaig visitar el laboratori del Prof. Baerends, ha influït decisivament durant la dècada dels anys 90 en la formació predoctoral i postdoctoral de diversos membres de l'IQCC i ha seguit fins ara a través d'una col·laboració continuada entre els dos grups de recerca.

El Prof. Baerends ha donat sempre suport als químics teòrics gironins, implicant-se en la seva formació i participant de manera molt destacada en els Girona Seminars de 2008 i 2010, reunions biennals organitzades per l'Institut. Ha contribuït de manera decisiva a millorar la qualitat de la recerca de l'Institut de Química Computacional i Catàlisi, del Departament de Química i de la Facultat de Ciències.

De les visites de membres del grup de recerca del Prof. Baerends a Girona destaquem les que va fer en diverses ocasions el mateix Prof. Baerends, o les de F. Matthias Bickelhaupt (en incomptables ocasions), de Célia Fonseca Guerra, de Ruud Visser, i de Marcel Swart quan era *postdoc* en el grup del Prof. Baerends. Membres del nostre Institut han visitat el grup de recerca del Prof. Baerends en diverses ocasions, com per exemple Jordi Poater com a doctorand i *postdoc*, Pedro Salvador, Marcel Swart, Sergei Vyboishchikov, Sílvia Simon, Anna Dachs, David Hugas, Laia Guillaumes, Juan Pablo Martínez, Abril C. Castro i un servidor, que vaig realitzar-hi una primera visita l'any 1994 que va marcar la meva carrera científica.

La relació del Prof. Baerends amb la Universitat de Girona ha estat llarga i intensa i ha donat com a fruit més de 60 publicacions conjuntes i múltiples presentacions a congressos, així com la signatura de diversos convenis. El primer d'aquests convenis va ser signat l'11 de gener de 2012 i regulava la col·laboració entre les dues Universitats en el camp de la Química Teòrica i Computacional. Dos doctors (Laia Guillaumes i Juan Pablo Martínez) ja han defensat la seva tesi cotutelada entre la Universitat de Girona i la Vrije Universiteit Amsterdam en base a aquest conveni.

El Prof. Baerends té una projecció molt important, doncs, de mestratge sobre diversos professors i investigadors del Departament de Química i de l'Institut de Química Computacional i Catàlisi. Val a dir que aquest mestratge s'ha estès a altres professors i investigadors d'altres universitats i centres de recerca catalans. Com a més destacades, podem mencionar les col·laboracions del Prof. Baerends amb els professors Vicenç Branchadell i Mariona Sodupe, de la Universitat Autònoma de Barcelona; amb el professor Josep Maria Poblet, de la Universitat Rovira i Virgili, i amb el professor Carles Bo, de l'Institut Català d'Investigacions Químiques.

Deixeu-me acabar amb un fragment del llibre *Ideas sobre la complejidad del mundo,* del professor Jorge Wagensberg, recentment traspassat, físic català i professor de teoria dels processos irreversibles a la Facultat de Física de la Universitat de Barcelona, expert en museologia i primer director del CosmoCaixa. Sobre la simulació científica, escriu Wagensberg: «El panorama de la investigación científica de vanguardia se ha visto conmocionado por los simuladores. Los científicos conocen bien el valor de un resultado experimental o de un resultado teórico, pero ¿cuál es el valor de un resultado simulado? Hay dos extremos que interesa comentar. El primero se refiere a aquellas teorías que tienen poca oportunidad de llegar a ser contrastadas con la realidad. Son los científicos ultrateóricos, tanto que a veces, y no sin ironía, se les conoce como los científicos-poeta. El drama aquí es una teoría sin experiencia. (...) La simulación ayuda a estos científicos-poeta porque ayuda a legitimar teorías. Ayuda menos que lo haría un experimento, de acuerdo, pero ayuda más que no tener nada. (...) En este caso, la simulación no es experiencia, pero hace de, la sustituye en relación con la teoría. El otro extremo se refiere a observaciones o experimentos que se nos antojan incomprensibles por incomprensibles, esto es, cuando no puede encontrarse ninguna teoría que sea más compacta que la propia observación. Para muchos científicos tales experimentos nada aportan en favor de la inteligibilidad de la realidad, no van más allá de la realidad, es decir, son sólo una buena cocina. Al científico-poeta se opone entonces, con similar problema, el científico-cocinero. El drama ahora es el de la experiencia sin teoría. La simulación también sirve de socorro en este extremo. Un experimento que converja con cierta simulación tiene más valor científico que un experimento que no converja con nada en absoluto. Aquí la simulación no es teoría, pero hace de, la sustituye en el sentido de que confiere una cierta inteligibilidad a cierta realidad. ¿En qué quedamos? ¿Es la simulación una especie de experiencia o una especie de teoría? (...) La simulación no es teoría ni experiencia, ni un mero útil de cálculo, sino una genuina forma de aproximación a la realidad que acaso esté revolucionando el mismísimo método científico.»

Com hem assenyalat en subratllar els mèrits científics del Prof. Baerends, aquest ha destacat tant en la vessant de químic-poeta, desenvolupant nova teoria no sempre confrontable amb resultats experimentals, i per tant necessitada de simulacions per ser legitimada, com en la vessant de químic-cuiner, portant a terme simulacions que han permès fer més comprensibles realitats químiques altament complexes. Però ha anat més enllà, i amb les seves simulacions ha aconseguit una comprensió profunda de l'enllaç químic. «Un cop s'entén l'univers a nivell atòmic, la resta és senzilla» va dir el Prof. Richard P. Feynman. Certament, les aportacions de Baerends ens han permès avançar en aquesta direcció i entendre millor el nostre univers als nivells atòmic i molecular.

El Prof. Baerends s'ha fet un lloc d'honor dins la potent escola holandesa de químics-físics, entre els quals hi ha figures com Johannes Diderik Henricus van der Waals (premi Nobel de Física 1910), Jacobus Henrikus van't Hoff (premi Nobel de Química 1901), Peter Joseph William Debye (Premi Nobel de Química 1936) o Paul Josef Crutzen (Premi Nobel de Química 1995). Isaac Newton va adaptar una frase atribuïda a Bernard de Chartres per dir: «He pogut veure més lluny que ningú perquè he pujat a les espatlles de gegants.» En el camp de la DFT, Baerends ha estat un d'aquests gegants que ha permès a molts químics teòrics i computacionals, entre ells molts membres de l'Institut de Química Computacional i Catàlisi, veure-hi més lluny.

Baerends ha estat una font d'inspiració permanent per a molts doctorands i *postdocs* que ha dirigit amb rigor i passió. Amb el seu mestratge el Prof. Baerends ha contribuït decisivament a la formació d'investigadors que han fet aportacions molt rellevants en el camp de la química teòrica, ha establert una xarxa de col·laboracions internacionals sòlida, i el que també és molt important, ho ha fet gràcies al seu esperit crític, un entusiasme sense fi, una capacitat de treball molt elevada i una motivació per treballar en equip envejable. Tot plegat ha contribuït a fer avançar la frontera de la ciència i a aixecar el nivell de la química teòrica europea i mundial.

És, doncs, per moltes raons i, certament, per tot això, Rector Magnífic, que sol·licitem que s'atorgui i es confereixi el grau de doctor honoris causa al Prof. Evert Jan Baerends.

Dr. Miquel Solà Puig

Dr. Marcel Swart

Girona, 9 de maig de 2019

Discurs del Dr. Evert Jan Baerends


Prof. Dr. Evert Jan Baerends

Esteemed Rector Magnificus,

President of the Board of Trustees of the University of Girona,

Esteemed Authorities,

Professors, Students and Members of the University Staff,

Ladies and Gentlemen,

It is a great honor for me to receive the doctorate honoris causa from your university. For several reasons.

One of the reasons is the special place that Catalunya has held for me since a long time. I think contacts started in the nineties when Dr. Miquel Sola, now professor Miquel Sola, spent time as a postdoc in Amsterdam. I spent three summer periods as an Iberdrola Fellow at the Universita Autonoma de Barcelona, being hosted by professors Joan Bertran, Mariona Sodupe and Vicenz Branchadell, renewing also contacts with the Theoretical and Computational Chemistry group of the University of Girona at that time. The contacts have not been limited to Universita Autonoma de Barcelona or Girona, I remember memorable visits to Tarragona and to the University of Barcelona. I cannot record all contacts, but I should mention that since that time a strong connection with the Netherlands has built up over the years, with many fruitful exchanges.

Another reason to enjoy this award, apart from the personal honor it brings to me, is the tribute it constitutes to the field of science I am involved with, and am representing today, namely chemistry. It is a truism that science in general, and chemistry and physics in particular, have shaped our modern world. Maybe I should include biology, and then in its wake also medical science, but let me note a bit chauvinistically that biochemistry has hugely impacted biology and medicine. It is not only the technical achievements of the natural sciences that have impacted our lives. Their influence is much broader and deeper. They shape our culture and our outlook on life. They also are a source of beauty. Chemistry offers the beauty of chemical structures. I just have to mention the DNA molecule, with its intricate double helix structure. And chemistry is a creative art. It creates many new beautiful structures, never before realized in nature.

On this occasion, however, I want to stress the lesson science teaches us about our mental outlook. Given that this award is in chemistry, in particular in theoretical chemistry, and then in the subfield of density functional theory, I think it is appropriate to highlight the role of open mindedness, the lack of prejudice, the flexibility of mind to adopt new paradigms, even when not yet completely established. In science, any preconception runs the risk of being thoroughly demolished. It appears that all obvious conceptions in whatever field one is interested in, are bound to be dispelled by further investigation.

By way of example, before I focus on theoretical chemistry, let me remind you of a very well known but actually very esoteric problem, that the most famous scientist ever has set himself. This most famous scientist is Einstein, you will agree. The question he struggled with is: can anything go faster than light? Isn't that an irritating question at a time the highest speeds were achieved by trains running ca. 100 km per hour, compared to the speed of light of 300 000 km per second? I am afraid a grant application by Einstein would not have been rated high at "usefulness for society".

Now we all know that Einsteins results have revealed staggering insights in such fundamental issues as the nature of space and time. But also position determination with GPS needs Einsteins theory of relativity. The utterly useful and very widely employed GPS devices that serve as the everyday navigation equipment in our automobiles rely on the theory of relativity! GPS has also revolutionized navigation at sea. Sextants and celestial navigation are not even taught any more at maritime schools! Often, the more fundamental insights are, the more revolutionary useful they prove to be. The lesson is: never reject a notion or question off-hand, however irritating or esoteric it may seem, be open minded and unprejudiced.

Let me focus then on chemistry, and to make a long story short, on my own field of the theory of chemical bonding and structure. Let me start with the picture of bonding by electron pairs as developed by Gilbert Lewis (Figure 1), which I think every high-school student will remember from his chemistry classes. In the first decades of the twentieth century Lewis pictured chemical bonds as arising from electron pairs (Figure 2), and the remaining electrons pairing up in so-called lone pairs. This model rationalized a large number of known facts. In the first place the predominance of compounds with an even number of electrons. In the second place the explanation within this model of the valences of the elements when combined with the rule that an atom tries to collect 8 electrons (the octet rule). But of course there is also something ridiculous in this theory: why would negatively charged electrons, which according to electrostatics will repel each other, get together to form a bond? Moreover, just at the time Lewis was developing these ideas, the Bohr theory of the hydrogen atom, which pictures electrons as fast moving particles circling the atomic nucleus, like planets are circling the sun, was astonishingly successful in predicting quantitatively the spectra of the H atom. In a sense Bohr's model marks the beginning of the efforts that would lead, about a decade later, to quantum mechanics. Quantum mechanics is one of the two great theories of physics to emerge in the twentieth century, and from the physics side there was only ridicule and contempt for Lewis's model. And not only from physics. Also many physical chemists felt that Lewis's electron pair theory was too simplistic, the basis of electronic structure theory should rest firmly in the quantum theoretical treatment of the motions of the electrons. This may have cost Lewis the Nobel prize, he is often referred to as the most famous and deserving chemist who never got the Prize. But we should recognize that Lewis has had enormous impact in chemistry. His concepts were so useful and such an excellent basis for theorizing about bonding in molecules that even today every chemist knows what Lewis structures are. Much of his thinking, for instance his generalization of the concepts of acidity and basicity, to donation and acceptance of electron pairs, are now fully vindicated by quantum chemistry. Lewis is another example that we should beware of hasty condemnation and be open minded and unprejudiced.

It has been Linus Pauling (Figure 3) who has done an admirable job of tying in quantum mechanics with Lewis's ideas, even before computers were powerful enough to actually perform quantum mechanical calculations on the motions of the electrons. He realized that even without computation one can give chemists a feeling for the relative importance of quantum mechanical effects by considering what he called "resonance" among various electronic structures. These contributions, also called valence bond structures, translate into simple pictures the quantum mechanical superposition principle (Figure 4). Many chemists who never studied quantum mechanics in any depth, and would think of it as a rather esoteric physical theory, were as a matter of fact practicing quantum mechanical concepts in their daily thinking and talking about the structures and reactivity of their compounds. I am ashamed to admit that as a young theoretical chemist I have made the error of ridiculing Lewis's and Pauling's models with their "unphysical" electron pairs, and the arrows indicating how these pairs might hop around in order to create other contributing resonance structures. So modesty is something that has to be acquired. We should be open minded and modest enough to keep in mind that what seems at first sight to be absurd and contrary to accepted wisdom may eventually turn out to contain a lot of truth.

Lewis and Pauling created a paper and pencil method for judging bonding and structures of compounds. But when computers became sufficiently powerful, it became possible to actually carry out the complicated and time-consuming calculations that are necessary to solve the quantum mechanical equations with sufficient accuracy. Sufficient accuracy was denoted "chemical accuracy", something like 0.1 kcal/mol in the energy. That would make it possible to actually do "chemistry on the computer" or "in silico". This development started slowly in the fifties and then made great leaps in the subsequent decades, mostly through the astonishing improvements in computer technology. Expectations (in my opinion unrealistic) were very high that eventually, maybe even soon, reducing chemistry to a computational science might become a reality. There was also a clear paradigm: calculations should be done "*ab initio*", that is by solving the equations purely by mathematical and numerical methods, without empirical parameters. We may use the picture of Thomas Kuhn, who distinguished periods of "normal science" and "scientific revolutions". In our case then, the paradigm was given, no scientific revolution would be needed. We could envisage a period of "normal science" where theoretical chemists would work hard on the given task of developing increasingly sophisticated and efficient techniques of solving the given equations. They would eventually reach the holy grail of "chemical accuracy".

As Kuhn describes, scientists usually enjoy such normal science. The goal is clear, it is easy to see who makes the smartest contributions to solving the set problem. All efforts can be directed towards developing methods to solve the given problem. No need to waste time and energy on debates about the underlying science or the goals to be reached. However, the downside is that the scientists no longer are so modest as to recognize that maybe the chosen path is not the right one, or at least not the only one. They may hate colleagues who will doubt the accepted paradigm, with a professional and sometimes even personal hatred.

This is what happened when in the seventies and eighties a new paradigm was provided in our science by the advent of density functional theory. We give it the acronym DFT. This is not the place to go into any detail about this theory. Let me just note that it provided a great simplification of the equations to be solved. The big drawback was the absence of a simple straightforward path to the exact solutions. In theory DFT did afford exact solutions. But often "in theory" is almost a euphemism for "not in practice". That is also to some extent the case with DFT, but not completely. It has not been made exact, by no means, but it is sufficiently accurate to be eminently useful. My career has entirely revolved around this particular approach. DFT has become thoroughly successful, by now maybe 90% of all quantum chemical calculations are DFT calculations. But the initial reception of DFT was utterly hostile. How did a small group of theoretical chemists dare to challenge the path forward that had been chosen by the very large majority of theoretical chemists, namely *ab initio* calculations? If I look back on my career, I like to divide it into two halves: the first twenty years (seventies and eighties) I was met, as a DFT practitioner and developer, with scorn and contempt. I remember a conference, organized by two well known professors in our field, in the mid eighties, where I was invited as a speaker. But they were harassing me so much at that meeting, that afterwards their students invited me to dinner, telling me how embarassed they were by this treatment. That is an illustration of the danger that old and established scientists are in. They may get too much entrenched in their pet theories and methods and may start to consider anything else as an aberration. It is also a beautiful illustration that, fortunately, young people tend to be much more open minded. That I am receiving this doctorate honoris causa today I consider a great honor for me personally, but at the same time I think it is recognition of the importance of the scientific revolution that has led to the predominance of DFT in our field, in particular for large systems.

But what I want to single out most is that again we see demonstrated that as scientists, we should never be rigid and prejudiced. We should be rigorous in our proofs and deductions, but that is a different matter. Things may always turn out to be just the opposite of what we think. Actually, they very often do. The *ab initio* approach looked so admirably clear and rigorous, while DFT was, and still is, far from straightforward and indeed somewhat muddled. Many people do not fully understand it, and there is still much to be criticized. But it has provided an enormous boost to the application of quantum chemical methods in chemistry. When I started my scientific career, most of the chemistry professors at my university, and surely at other universities as well, would question any "chemical relevance" of the theoretical chemists, with their penchant for mathematics and physics and computer work. That attitude amongst experimental colleagues has totally disappeared. They now enjoy to have computational input to their work. That is almost hundred percent owing to DFT.

So DFT is my last and telling example of the great virtue and even necessity in science to be open minded and without prejudice. It gives me great joy and satisfaction that this award underlines how this principle can lead, as so often in history, to unexpected and important progress.

Thank you for your attention.

Evert Jan Baerends,

Girona, May 9, 2019


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Nitrate ion
Universitat de Girona
Facultat de Ciències


Prof. Dr. Evert Jan Baerends
ersitat de Girona
ltat de Ciències

Presentació del Dr. Sovan Lek a càrrec del Professor Emili García-Berthou

Honorable Rector,

Distinguished Authorities,

Colleagues from the university community,

I will speak in English so that Professor Lek and the several people accompanying him will understand me, and then I will briefly summarize some of what I have said in Catalan. It is an honor and a privilege for me to summarize, in this solemn academic session, the merits of Professor Sovan Lek on this occasion granting him an honorary doctorate from the University of Girona promoted by the Department of Environmental Sciences.

Sovan Lek was born in 1952 in Cambodia. As you know, Cambodia lies between Thailand and Vietnam in Southeast Asia. It is famous for the temple complex of Angkor Wat, a UNESCO World Heritage Site built by the Khmer Empire during the 12th century. Sadly, Cambodia is also known for the Cambodian genocide committed by the Khmer Rouge, which killed more than 1.5 million people from 1975 until 1979. Professor Lek was fortunate to have obtained a B.Sc. from the University of Phnom Penh in 1974, the year before the genocide, and moved to France to pursue further studies. He obtained a M.Sc. in Hydrobiology from the University Paul Sabatier, in Toulouse (France) in 1975, and in 1978 a Ph.D. in Hydrobiology from the University Paul Sabatier under the supervision of Christian Lévêque. His Ph.D. thesis was on the biology and ecology of small characiform fishes in Lake Chad, Africa. He was an assistant professor at the University of Algiers in Algeria from 1979 to 1983 and an assistant professor at the University of Meknes in Morocco from 1983 to 1989. After that, he joined the University Paul Sabatier (Toulouse III) with his wife, Sithan Ang-Lek, who is also an ecologist and is with us here today. They spent the rest of their scientific careers in Toulouse. Sovan Lek was named a Distinguished Professor (*Professeur de Classe Exceptionnelle*) at the University of Toulouse and is now a Professor Emeritus.

Professor Lek's research has focused on the community ecology of freshwater fish and ecological modeling. Within community ecology, he has added to the understanding of how environmental factors and human perturbations, such as climate change or reservoirs, affect inland fish. Freshwater fish will undergo many changes because of climate warming and many factors. Climate change will affect water availability and the flow regime of rivers. What is more, freshwater fish dispersal is generally limited within river basins and they cannot easily adapt to climate change, and most freshwater organisms are ectothermic, or cold-blooded, and the ecological functioning of freshwater ecosystems depends markedly on temperature. Professor Lek has co-authored several of the best papers modeling the likely future effects of climate change on freshwater fish in Europe. He and his colleagues have shown that the habitats of cold-water species will decrease and may even disappear from many river reaches, whereas other species will shift their distribution, changing the overall structure of ecological communities. Professor Lek has also published many papers on the current and future ecological effects of dams and reservoirs, which are very important to society. They provide water for human consumption, irrigation and industries; they regulate floods and generate electricity. However, dams also have huge environmental impacts: they completely alter rivers' flow regimes, sediment and temperature regimes, ecosystem functioning, connectivity, and the extent of their flood plains, riparian ecosystems and wetlands. They change everything. Like our research group, Professor Lek has shown that small hydropower dams in the Pyrenees change flow regimes and affect the abundance of brown trout. He has also shown that in some of the world's largest rivers, such as the Mekong River, which starts in China and crosses Southeast Asia, dams disrupt natural seasonal river pulses, decrease species diversity, homogenize fish faunas, and favor generalist species. He has also led some large research projects in Tonle Sap Lake, which is the largest natural lake in Southeast Asia and constitutes one of the world's largest fisheries, supporting the livelihood of millions of people. Tonle Sap Lake is known for its flood-pulse character, affected by fish over-exploitation and dam construction in the Mekong River, where many hydropower reservoirs are being built or planned, like in many regions of the world, particularly in the tropics.

Professor Lek's other main research topic is machine learning and the application of advanced modeling techniques to ecological data. His three most cited papers, published in the journal *Ecological Modelling*, are on the application of artificial neural networks. According to Professor Lek, artificial neural networks are intelligent, thinking machines, developed from artificial intelligence and working in the same way as the animal brain. They learn from experience in a way that no conventional computer can and they rapidly solve difficult computational problems. In the 1990s, Professor Lek pioneered the application of artificial neural networks in ecology, in a time when they were much more difficult to apply than they are now. Artificial neural networks are now used routinely in speech or image recognition, in chemical or biomedical research. Professor Lek has edited several books that deal with these modeling techniques, but most notably two: *Artificial Neuronal Networks: Application to Ecology and Evolution* (published in 2000) and *Modelling Community Structure in Freshwater Ecosystems* (published in 2005). Although Sovan Lek has over 250 international publications that have received many thousands of citations, many other aspects of his scientific career are important. Professor Lek has taught for his entire career mostly in Toulouse and, in recent years, he has provided many free courses in his home country, Cambodia. He has advised many students, and has obtained funding for and coordinated several European projects. He has also participated in university management (for example, director of a school of doctoral studies in Toulouse). We often forget that an academic career is much more than publications and that many other aspects, such as teaching, supervising, coordinating research groups, university management, editorial work and peer review, or outreach, are equally important. In all these aspects, Professor Lek has made many important contributions.

Nevertheless, perhaps a more decisive reason behind his nomination for an honorary degree was his leading work on many Erasmus Mundus and Erasmus+ projects of the European Commission, some of which including the University of Girona as a partner. Erasmus Mundus partnerships were cooperation and mobility programs between European and third country higher education institutions (mostly from developing countries) that included scholarships and mobility fellowships. In recent years, they have been replaced by Erasmus+ actions. Professor Lek has conceived, obtained funding for and participated in about nine Erasmus Mundus and Erasmus+ projects, five of them involving the University of Girona (UdG). I was very fortunate to participate in three of them as coordinator at the UdG: TECHNO, TECHNO II, and NESSIE. Thanks to these three projects, led by Professor Lek, Jean-Michel Baleynaud, and Georges Zissis, respectively, the UdG received over a million euros so that about 75 students and academics could come to Girona, mostly from Asia. They included about 28 Cambodians, 8 people from China, 5 from Laos, 5 from Vietnam, 4 from Thailand, 3 from Malaysia, 2 from Indonesia, and 1 from Mongolia. They came to UdG to complete all kinds of studies or stays: at the undergraduate, master, doctoral or postdoctoral levels, or as staff. Many Asian students have obtained their master's or Ph.D. degrees at the University of Girona and are now back their home countries to share their education and research skills with newer generations and to continue their relationship with the UdG. Thanks to the NESSIE partnership, 16 UdG researchers visited New Zealand or Australia, and some researchers from Korea, New Zealand and Australia stayed in Girona. I would like to take this opportunity to thank the many people from the UdG who have helped considerably in these partnerships, notably Raquel Solà, Laura Ripoll, and others in the External Relations Office, Patricia Eyskens, then at the Polytechnic School, and many academics including Dr. Albert Turón, Dr. Quim de Ciurana or Dr. Gerard Arbat. Although for me these partnerships entailed a lot of work that is not necessarily valued in academia, they were a real milestone in my career and enriched my personal experience. They were rewarding in terms of learning about new cultures and landscapes and helping people. I know that they were enriching for many other UdG staff and in particular for the many Asian people involved. The Erasmus Mundus partnerships were eventually replaced by Erasmus+ actions. Dr. Helena Guasch at the UdG recently led one called UNICAM to implement a master's of science in sustainable agriculture in Cambodia. In addition, Professor Lek is leading one called CONSEA to implement a master's program in aquatic biodiversity and conservation and a Ph.D. program in sustainable ecosystem management in Southeast Asia, also with the participation of the UdG, coordinated by Dr. Anna Vila-Gispert. All these partnerships and actions were promoted and made reality largely by Professor Lek, who opened many doors of Asia to the UdG. Cambodia is still one of the world's poorest countries (among the 47 least developed countries, according to the United Nations) and an important motivation of Prof. Lek's activity has been always to improve Cambodia's educational and research quality and to give back to his home country what he obtained in France. Certainly, he has unselfishly succeeded in doing so and, at the same time, has benefitted Girona and its university.

I ara, el breu resum en català. El professor Lek ha publicat més de 250 treballs en revistes internacionals, sobretot en ecologia de comunitats de peixos continentals i en l'aplicació de tècniques noves d'anàlisi, com ara les xarxes neuronals artificials, a les dades ecològiques. Però també té moltes altres contribucions tant o més importants, com ara la millora de la recerca i del coneixement ambiental en països en desenvolupament com Cambodja, el seu país d'origen. També ha promogut, i en bona part liderat, nou projectes Erasmus Mundus i Erasmus+, en cinc dels quals ha participat la Universitat de Girona. Gràcies a aquests projectes la UdG ha rebut més d'un milió d'euros amb els quals més de 75 estudiants o acadèmics asiàtics han vingut a la UdG per tal de fer estudis de grau, postgrau o recerca, i més de 16 investigadors de la UdG han fet estades a Àsia, Austràlia i Nova Zelanda.

Aquest doctorat honorífic també és oportú perquè el govern català va aprovar que el 2019 celebrem oficialment el centenari del naixement del professor Ramon Margalef, un altre ecòleg, i perquè cada any el dia 9 de maig, com avui, és la Diada d'Europa. Ramon Margalef és àmpliament considerat l'ecòleg més influent que l'Estat espanyol ha tingut i un altre exemple, com el professor Lek, que tot i que les publicacions internacionals són el producte principal d'investigació dels científics, hi ha altres aspectes encara més importants per ser molt influents, com ara els llibres, la supervisió d'estudiants, l'ensenyament universitari, la col·laboració internacional i la transferència de coneixement. Els professors Margalef i Lek són també exemples que la investigació ambiental i ecològica és més important que mai en un món canviant, que té molts problemes ambientals i socials. Amb aquest doctorat honoris causa al professor Lek, la Universitat de Girona celebra el centenari del naixement del professor Ramon Margalef i ajuda a reconèixer la importància de la cooperació i l'educació universitària als països en desenvolupament, la col·laboració europea i internacional, la recerca ambiental i la conservació de la biodiversitat. És, doncs, per tot això, Rector Magnífic, que sol·licito que s'atorgui i es confereixi el grau de doctor honoris causa al professor Sovan Lek.

Dr. Emili García-Berthou

Girona, 9 de maig de 2019

Discurs del Dr. Sovan Lek

Distinguished Rector of the University of Girona;

Distinguished academic, political and civil authorities;

Colleagues from the university community;

Dear students;

Ladies and gentlemen;

I am honoured to be in the Honoris Causa list of UdG and I am very happy to be present in this solemn academic ceremony.

Let me first give detail about my origin. My father was born in South China in 1916. In 1940, China was in great crisis of insecurity (my grandfather was murdered, his body never found) and lack of food. My father, aged 24, migrated to Cambodia. I was born in 1952 in Cambodia, the 3rd of 9 in the family. In 1974, I left Cambodia to do the PhD in Toulouse for 3 years (I got a scholarship from the French government). When I finished my PhD in 1978, it was the Khmer-rouge and Pol Pot regime in Cambodia, and I did not return and always stayed in Toulouse up to now! With my wife (present here), we had 2 sons (born in France in 1977 and 1980). Both are aeronautical engineers, linked probably to our life in Toulouse. One son decided to leave France to Canada for 3 years in 2011 to have international experiences. But he still stays there and got last year Canadian citizenship. Now, I have 1 grandson and 1 granddaughter born in Canada. So, we are really global citizens!

I had the chance to be integrated at the University Paul Sabatier (Toulouse III) as full Professor. I had the opportunity to set up the aquatic research team namely AQUAECO within the laboratory "Evolution &

Biological Diversity". AQUAECO accounts now for more than 10 permanent staffs including University Professors but also researchers from CNRS and IRD (Institute for Research & Development).

My researches focus on Fish community, especially to the change of Biodiversity in the context of the changing world, including climate change and global environmental changes.

Biodiversity such as species richness, i.e. the number of species living in the specific area, is strongly impacted by the modern life. Understanding the mechanism of the biodiversity changes in the context of the changing world is very important.

My research focuses especially to the development of the efficiency statistical methods that can predict the biodiversity changes in space and time. For example I have used ANN (artificial neural networks) to predict Fish Species richness worldwide. At the global scale, fish diversity is different from one place to another place. For example, there are thousands species living in Amazon, only 20-30 species in Ebro and most of them are introduced species. ANN models can predict perfectly these changes from only a few parameters, and we found that Primary productivity is the most important parameter explaining the change of fish diversity. So, the high richness of fish in Amazon, Congo, Mekong,... is explained not only by the big area, but also the high productivity. The decrease of productivity due to changes of the environment (e.g. deforestation, climate change) can strongly affect diversity of fish.

At the smaller scale, I contributed to several EU projects on the aquatic biodiversity to predict fish biodiversity in the context of climate change and aquatic contaminants (for example effect of pesticides on fish populations). By using machine learning, especially Ensemble modelling, it is now possible to predict changes in fish diversity in streams in the future (e.g. year 2080, 2100). The results show that the fish species in our rivers will change a lot in the future due to climate change, in term of species richness, turnover and abundances.

Due probably to my origin, during the last recent years, I have also contributed my research in China and South-East Asia as freshwater fishes are very important in food consumption, and the environmental impacts are very important, e.g. damming, overfishing, pollution... In China, Yangtze (3rd world largest river) is strongly impacted by the cascade dams, especially the Three-Gorges dam, one of the largest dams (200 m high, 22 500 MW energy). My works focus mostly to preserve diversity in river dominated by endemic species. The Mekong is an international river crossing several countries (China and several countries in SEA) that has high fish abundance and diversity. But the Mekong is strongly impacted by overfishing and all other human activities (pollution, dam, climate change...). Recent research results show clearly decreasing fish abundance, diversity as well as fish size! The challenge is to preserve the diversity and abundance of fish in this river for future generations.

Between Girona and Toulouse, we need only 3 hours drive, i.e. more or less the same distance than Toulouse to Bordeaux or Montpellier, but much shorter than Lyon or Paris... Girona is in Catalogna and Toulouse in Occotania, very close culture each-other. So, it can explain that there has always a lot of cooperation between Girona and Toulouse in several fields. My collaboration with UdG is quite ancient. I met Sergi Sabater early 1990 in Toulouse during a PhD defense on periphyton, and he told me about his colleague Emili García-Berthou who is fish ecologist that I immediately made contact!

From this date, we started our collaboration with participation in research projects and the jury of several PhD in both sides. The exchanges quickly expanded to the cooperation between the entire AQUAECO team in Toulouse and entire Institute of Aquatic Ecology team in Girona. Some examples:

- Emili has collaborated with several researchers in AQUAECO as Julien Cucherousset, Sébastien Brosse, Gael Grenouillet, Bernard Hugueny... They contribute currently to Biodiversa project ODYSSEUS that aims to study the effects of the Anthropogenic fragmentation on freshwaters fish;
- Pablo Tedesco has stayed in UdG as post-doc in 2006-2007, and he is now IRD researcher in AQUAECO;

– I have several collaborations with other member of the Institute of Aquatic Ecology in UdG. I contributed with Helena Guasch-Padró to MODELKEY project with EU 6th FP focusing on Aquatic ecotoxicology. Helena has also coordinated KeyBioEffects, a Marie-Curie project that allowed us to have some joint-PhDs between UdG and Toulouse III.

– In 7th FP, we got success with several Erasmus-Mundus projects TECHNO I & II that allowed UdG and UT3 to host several Master and PhD students, and Staff from Asian countries (China, Cambodia, Mongolia, Thailand, Vietnam. The NESSIE project allow us to open our cooperations to South Korea and Oceania (NZ and Australia).

– In Horizon 2020 Helena coordinated a Erasmus+ Capacity Building project UNICAM... With Marta MUÑOZ-FRIGOLA and Anna VILA-GISPERT, we contributed to another Capacity Buiding CONSEA project coordinated by Toulouse.

– ...

These examples show the importance of the cooperation between Aquatic Ecologists in Girona and Toulouse. We succeeded to create a large research network with other European Universities and other countries in the world to improve our research capacity for Aquatic ecology, and train the young researchers worldwide. I hope that our effort will be important for the conservation of the biodiversity especially in the aquatic ecosystems.

The best honour for a university teacher and researcher is that which comes from the appreciation of his colleagues in the world-wide academic republic. By granting me a Doctorate honoris causa at your university you have done me that honour, and my first duty is to thank the University of Girona for allowing me to receive this precious gift. I say ‘the University’. But a University itself does not make such decisions. They are proposed by one or more individuals, supported by others, and finally approved and promulgated by those who represent the full authority of the University. They are all real people, not formal institutions and I would like to thank all of them personally as well as collectively for what they have done to give me this honour, as well as to thank them for arranging the journey in this beautiful and historic city.

It is a pleasure and an honour to receive a degree h.c. from the University of Girona.

Thank you very much, University of Girona!

Moltes gràcies a la Universitat de Girona.

Sovan Lek

Girona, May 9, 2019


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Investidura Doctor honoris causa
Evert Jan Baerends
Sovan Lek

Discurs del Dr. Quim Salvi Mas


VNIVERSITAT
DE GIRONA
EL RECTOR

Distinguished doctors,

President of the UdG's Board of Trustees,

Director of the School of Doctoral Studies,

Directors of the Departments of Chemistry and of Environmental Sciences,

and Director of the Institute of Computational Chemistry and Catalysis, sponsors of the honorary doctorate recipients, and friends,

Universities are institutions shaped by a wide variety of historical, territorial, economic and social factors. Established to increase and transfer knowledge, they cannot avoid certain obligations. These include providing training that contributes to social progress and improves conditions for students; conducting research to deepen and widen our knowledge of the world and of how this knowledge influences our well-being; and being involved in sustainable development and in the struggle against inequality.

And much more than that.

However, there comes a time, a precise moment, in which universities, aware of all these obligations, also demonstrate what they are and what they represent: an authentic measure of their characters.

In one of the more solemn ceremonies celebrated during the academic year, the University of Girona does the same. By awarding honorary doctorates, the University defines and reaffirms its values, pays tribute to the individual persons who have made it what it is, and recognises their accumulated merits. Awarding honorary doctorates is proof of the University's respect and admiration and a way of demonstrating that to the world.

The University is also, and to an extraordinary degree, all the persons – men and women – who have earned the most important degree awarded by our institution. The honoris cause doctorate ceremony is one of great institutional significance.

The University welcomes, as one of its own, a person or persons who have excelled in their personal lives and professional careers and whose achievements have benefitted the University, with which they have maintained a close, productive and ongoing relationship.

The University's honorary doctorate recipients include psychologists, chemists, singers, historians, economists, philosophers, geologists, physicians, legal scholars, politicians, chefs, intellectuals, writers, ichthyologists, educators, physicists, poets and health professionals. These men and women have, in one way or another, contributed to progress in the sciences, the humanities and society.

Today we expand this list of honourees to include two renowned professors, recognised worldwide, from the field of science.

Through their work and masterful teaching, they have contributed, not only to scientific progress in the fields of chemistry and ecology, but also to the University of Girona's reputation as a leading research institution open to international collaboration.

We have already drawn attention to their merits. I can only add, in the name of the University, our congratulations and our deepest and most sincere gratitude for your relevant academic work.

The University's most recent honoris cause doctorate recipient, the poet Narcís Comadira, once said, "Universities are the future of our country". With ceremonies like this, we reaffirm that purpose. It is achievable if we all work toward it. Today, with two new honorary doctors, we have more reasons, more hope, more support to meet the challenge.

To Doctor Evert Jan Baerends, who unfortunately cannot be with us today, and to Doctor Sovan Lek, for whose presence I am very grateful, thank you very much.

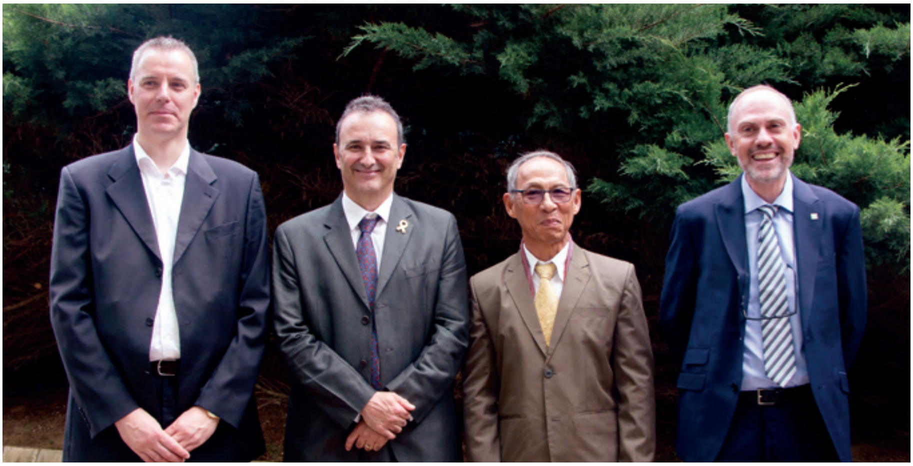
The University community welcomes you with enthusiasm and is eager to continue our collaboration. The University of Girona is your home.

Thank you,

Quim Salvi

Rector

Girona, May 9, 2019




Sovan Lek
Dr. Sovan Lek
Facultat de Ci

Universitat de Girona