Proposta de nomenament del Prof. Dr. Evert Jan Baerends com a Doctor Honoris Causa per la Universitat de Girona

1. Presentació
2. Acord del Consell del Departament de Química
3. Acord d'adhesió del Consell de l'Institut de Química Computacional
4. Memòria en relació al punt VII de la normativa d'ordenació dels ensenyaments universitaris de doctorat de la Universitat de Girona aprovada pel Consell de Govern en la sessió 3/12, de 26 d'abril de 2012
    a. Mèrits científics
    b. Projecció de mestratge
    c. Relacions amb la UdG
    d. Curriculum vitae complet (en anglès)

Girona, novembre de 2013
Departament de Química

1. Presentació

El Prof. Dr. Evert Jan Baerends és un dels investigadors més destacats en el camp de la química teòrica i computacional actual. Va ser ell que en els anys 70 va iniciar un seguit d'estudis que van permetre el desenvolupament de la teoria del funcional de la densitat tal com la coneixem avui en dia. Sense el seu treball pioner no disposaríem avui d'una eina tan essencial per la química computacional com és la teoria del funcional de la densitat. A més, amb el seu mestratge el Prof. Baerends ha contribuït decisivament a la formació d'investigadors (molts d'ells lligats a l'Institut de Química Computacional i Catàlisi de la Universitat de Girona) que han fet contribucions 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 alta, 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 important destacar que el candidat ha contribuït decisivament a la formació i consolidació de vàries de les persones que actualment formen part del Departament de Química i de l'Institut de Química Computacional i Catàlisi (IQCC). La col·laboració que fa quasi vint anys es va iniciar quan el Dr. Miquel Solà va visitar el laboratori del Prof. Baerends ha influït decisivament durant la dècada dels anys 90 en la formació predoctoral i postdoctoral de varis membres de l'IQCC i ha continuat fins l'actualitat mitjançant 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 destacada en els Girona Seminars, reunions bianuals organitzades per l'IQCC. A ell li devem, per tant, part del mèrit d'haver contribuït 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.

Per un altre cantó, el Prof. Baerends ha contribuït enormement al progrés de la química teòrica mundial, en el camp de la teoria del funcional de la densitat, combinant el desenvolupament de nova metodologia amb l'aplicació a problemes d'interès químic. La seva gran capacitat d'entendre profundament la base dels fenòmens fisicoquímics i el seu entusiasme desbordant l'han acompanyat al llarg de tota la seva carrera professional i una prova en són els recents desenvolupaments que ha realitzat en el camp de la teoria del funcional de la densitat depenent del temps i en la recerca de nous funcionals. Un dels aspectes més destacats de la seva carrera és que ell va ser qui originalment va dissenyar el programa Amsterdam Density Functional (ADF) que actualment utilitzen per la seva recerca els laboratoris de química computacional més importants del món, tant a nivell acadèmic com empresarial.

La tasca realitzada en els últims 35 anys pel Prof. Baerends ha estat reconeguda internacionalment per moltes persones. A tall d'exemple podem destacar el seu fitxatge per la Universitat de Pohang a Corea del Sud com a "*World Class University Distinguished Professorship*" i per la Universitat King Abdul Aziz de Jeddah a Aràbia Saudi. També l'any 2001 se li va concedir la prestigiosa medalla Schlumberger i el 2010 la prestigiosa Schrödinger Medal de la World Association for Theoretically Oriented Chemists (WATOC). En canvi, ens sembla que no ha estat reconeguda suficientment per les Institucions europees (excepte evidentment per la seva pròpia universitat, la Vrije Universiteit, que el nomenà Professor Emèrit). La Universitat de Girona, per l'especial relació que hi ha tingut i que hi segueix tenint, és especialment idònia per fer-li un reconeixement a nivell català, espanyol i europeu.

I per això, el Departament de Química, amb l'adhesió de l'Institut de Química Computacional i Catàlisi, ha considerat adient proposar que se li atorgui el Doctorat Honoris Causa.

2. Acord del Consell del Departament de Química

El Consell del Departament de Química reunit el dia 27/01/2014 en sessió ordinària 1/14 ha acordat per assentiment aprovar la presentació del Prof. Baerends com a candidat a doctor honoris causa per la Universitat de Girona.

Acord unànime d'adhesió del Consell de l'Institut de Química Computacional i Catàlisi

El Consell de l'Institut de Química Computacional i Catàlisi reunit el dia 13 d'octubre de 2009 ha acordat adherir-se a la sol·licitud del Consell de Departament de Química de concessió del Doctorat Honoris Causa al Prof. Evert Jan Baerends.

3. Memòria en relació al punt VII de la normativa d'ordenació dels ensenyaments universitaris de doctorat de la Universitat de Girona aprovada pel Consell de Govern en la sessió 3/12, de 26 d'abril de 2012

4.a Mèrits científics

Breu Currículum Vitae
Nascut el 17/09/1945.
Llicenciat en Ciències Químiques (cum laude), Vrije Universiteit Amsterdam, 1967.
Estudis doctorals en Ciències Químiques (cum laude), Vrije Universiteit Amsterdam, 1967-1970.
Becari/Tesi doctoral, Vrije Universiteit Amsterdam (Dr. P. Ros), 1970-1975.
Doctor en Ciències Químiques (cum laude), Vrije Universiteit Amsterdam, 1975.
Postdoc a la Vrije Universiteit Amsterdam (1975-1976).
Professor Associat de la Vrije Universiteit Amsterdam (1976-1981).
Catedràtic d'Universitat, àrea de Química Teòrica, Vrije Universiteit Amsterdam (1981-2010).
Professor Emèrit, Vrije Universiteit Amsterdam (2010-).
Professor visitant contractat com a "World Class University Distinguished Professorship", Pohang University of Science and Technology, Corea del Sud (2009-2013).
Professor adjunt al Departament de Química de la King Abdul Aziz University, Jeddah, Saudi Arabia (2011-).

Camps UNESCO: 230701-230703-230723-221003-221001-221002-230321

Línies de recerca:

Teoria del funcional de la densitat per sistemes multielectrònics
Desenvolupament i aplicació de noves tècniques computacionals especialment en els programes ADF i BAND.
Estudis d'estructura electrònica i molecular, propietats moleculars, enllaç químic i reactivitat química
Desenvolupament de la teoria DFT depenent del temps amb aplicacions a l'estudi de propietats elèctriques, intensitats Raman, espectres electrònics i dicroïsme circular vibracional
Efectes relativístics en la química i espectroscòpia d'elements pesats
Estudi de les interaccions entre les molècules i les superfícies.
Teoria del funcional de la densitat matricial

- 34 tesis doctorals dirigides o codirigides
- 426 articles publicats en revistes internacionals

Premis
Unilever student award, 1970
Koninklijke/Shell Price, 1976
Member of the International Academy of Quantum Molecular Science, Juliol 1999

Recipient of Schlumberger Medal, Juny 20, 2001, Cambridge, UK
Membership Royal Netherlands Academy of Science, 2004
Schrödinger Medal, World Association for Theoretically Oriented Chemists (WATOC), 2010.

Citacions/Impacte: Aprox. 426 publications, índex h: 81.
Citations: 37545; Mitjana per article: 87.
Llistat a l'ISI Web of Science's website http://isihighlycited.com/ com un dels autors més citats dels darrers 25 anys.
Llistat al Royal Society of Chemistry's website
http://www.rsc.org/chemistryworld/News/2007/April/23040701.asp
com un dels químics vius més citats del món i el més citat d'Holanda.
Llistat en el top-100 dels químics més citats en el darrer període de 10 anys: Nov. 2005, Nov. 2006, Nov. 2007.

Professor visitant: Universität Konstanz, Germany, 1988.
Universität-Gesamthochschule Siegen, Germany, 1986.
Università Basilicata, Potenza, Italy, 1990.
Switzerland (Geneva, Lausanne, Fribourg) for lectures in the Convention Intercantonale Romande pour l'Enseignement du 3e Cycle en Chimie, sept. 1993.
University of Fribourg, Switzerland, 95/96.
Iberdrola Foundation visiting professor at Universitat Autònoma de Barcelona, juny-agost 1996.
Universitat Autònoma de Barcelona, juliol 1997 i juliol 1998.
University of Auckland, New Zealand, abril 1998.
Schlumberger Professor a la Cambridge University, UK, 2001, 2002, 2003.
Switzerland (Geneva, Lausanne, Fribourg) com a conferenciant en la Convention Intercantonale Romande pour l'Enseignement du 3e Cycle en Chimie, Nov. 2002.
Université Pierre et Marie Curie, Paris, France, 2005

Editor: Advisory Editorial Board Theoretical Chemistry Accounts, 1997-.
Advisory Editorial Board Physical Chemistry and Chemical Physics,1998-2001.
Advisory Editorial Board, Chemical Physics Letters, 2001-.
Advisory Editorial Board PhysChemComm 2002–2003.
Member Editorial Board Journal of Computational Chemistry 2004-.
Editorial board Research Letters in Physical Chemistry 2009-.

El camp científic del Prof. Baerends

La química quàntica, en subministrar una descripció rigorosa dels fenòmens químics, permet avançar en la seva interpretació i també preveure nous fenòmens. L'evolució de la informàtica ha permès amplificar la potència intel.lectual de l'home de forma anàloga a com la revolució industrial havia incrementat la seva potència física. Gràcies als ordinadors actuals, el càlcul teòric sobre un fenomen químic pot ésser competitiu amb l'experiment, i moltes vegades més ràpid i fins i tot més acurat. Aquesta competitivitat augmenta constantment per raons econòmiques, ja que mentre les despeses experimentals pugen cada dia, les de càlcul segueixen el procés contrari. El químic experimental compta amb una potent eina per orientar la recerca al seu laboratori, però el químic teòric també compta amb un laboratori, el de la simulació pura, on hi pot desenvolupar els seus experiments virtuals amb l'únic límit de la imaginació i la intuïció.

La faceta més característica del candidat ha estat la de desenvolupar la teoria i implementar la metodologia del que ha estat la revolució més gran en el camp de la química teòrica i computacional de finals del segle XX i principis del XXI, la teoria del funcional de la densitat. Cal dir que a l'any 1998, el fundador d'aquesta teòria (Prof. Walter Kohn) va rebre el Premi Nobel. En aquest sentit una de les aportacions més importants ha estat demostrar com és possible determinar el potencial de correlació-bescanvi exacte a partir d'una densitat exacta calculada amb un mètode full-CI. També ha contribuït de manera decisiva al desenvolupament de la teoria del funcional de la densitat matricial i a la teoria del funcional de la densitat depenent del temps. Ha estat el principal autor i impulsor dels programes Amsterdam Density Functional (ADF) i del BAND molt usats arreu del món per l'estudi de l'estructura i reactivitat de les espècies químiques.

L'entusiasme del Prof. Baerends i les seves ganes de comprendre els processos químics amb la metodologia provinent de la física s'han contagiat a molts de científics químics de Catalunya que han pogut contribuir, cadascun en el seu àmbit, en l'avenç de la frontera del coneixement. I ha fet, en particular, que a la Universitat de Girona hi hagi un grup de recerca de qualitat que es pugui comparar amb els altres catalans i que sigui un pol d'atracció per a investigadors de química teòrica de tot el món.

Els indicadors de qualitat

El Prof. Baerends és un dels químics teòrics i computacionals més citats del món tal com ho demostren les dades del "*Web of Science*" i els "*Essential Science Indicators*" tots dos de l'Institute for Scientific Information. En concret segons el "*Web of Science*" (dades de 27 d'agost de 2013) el Prof. Baerends ha publicat entre els anys 1972 i juliol de 2013 426 articles que han rebut la impressionant xifra de 37545 cites, el que representa que cada article ha estat citat 87 vegades. Té un índex h de 81, el que vol dir que té 81 articles que superen les 81 cites. De fet un del seus articles supera les 3150 cites i fins a 13 articles seus superen les 500 cites. Apareix en els "*Essential Science Indicators*" com a científic "significativament citat". De fet en els 10 anys que van del febrer 1999 al febrer 2009 segons aquesta base de dades havia publicat 150 articles que han estat citats 6097 vegades. Això el col·locava en la posició 145 entre els químics més citats del món i en la *sisena* posició entre els químics teòrics i computacionals més citats dels món, per davant d'il·lustres personatges en aquesta disciplina com ara H. F. Schaefer III, W. A. Goddard, M. H. Gordon, S. Shaik, G. E. Scuseria, K. S. Houk, P. v. R. Schleyer i tants altres. Només un químic espanyol, el Prof. Avelino Corma, es trobava per davant del candidat, en la posició 44. Els anys 2005, 2006 i 2007 va aparèixer en els "*Essential Science Indicators*" entre els 100 químics més citats del món. El seu nom surt llistat a la pàgina web http://isihighIycited.com/ del ISI Web of Science entre els científics més citats els darrers 25 anys. També apareix a la web de la Royal Society of Chemistry

http://www.rsc.org/chemistryworld/News/2007/April/23040701.asp com un dels químics vius més citats del món. Finalment dir que 11 dels 150 articles que ha publicat aquests 10 anys estan a la llista dels considerats "*highly cited papers*".

Principals mèrits científics

El Prof. Baerends al llarg de la seva carrera científica ha fet contribucions de gran importància al desenvolupament de la química teòrica i computacional. Possiblement la contribució més important ha estat al desenvolupament de la teoria del funcional de la densitat (DFT). Aquesta teoria és la que s'usa actualment en l'estudi de l'estructura i la reactivitat química en un percentatge altíssim dels articles publicats pels químics teòrics i computacionals. L'ús d'aquesta teoria de manera generalitzada es va produir a principis dels anys 90 quan els autors del programa Gaussian varen incloure la possibilitat d'usar DFT en aquest programa. Abans, però, hi va haver gent pionera que va desenvolupar la teoria DFT i va demostrar la seva validesa per l'estudi computacional de problemes d'arrel química. El Prof. Baerends va iniciar la seva recerca en la teoria DFT a principis dels anys 70, pocs anys després de la formulació dels teoremes de Hohenberg i Kohn que representen la base de la teoria DFT. Es tracta per tant d'un dels grans pioners en aquest camp i un dels científics que han fet aportacions més rellevants. Això és un fet reconegut internacionalment per tota la comunitat de químics teòrics i computacionals. De manera més detallada les seves grans aportacions a la química teòrica i computacional han estat:

1. Desenvolupament del programa de càlcul ADF basat en quatre grans ingredients: a) L'expansió estàndard dels orbitals Kohn-Sham en funció de bases de càlcul; b) L'ús de funcions de Slater pel càlcul; c) L'ús de bases auxiliars per reduir el cost del càlcul de la interacció Coulòmbica (ajust de la densitat o resolució de la identitat); d) La integració numèrica dels elements de la matriu Hamiltoniana. L'ajust de la densitat és una tècnica que permet reduir dràsticament el cost del càlcul de la interacció Coulòmbica i que ha estat adoptada per la major part de codis moderns de càlcul basats en la teoria DFT. De fet, a l'any 1994, inspirats per aquest resultat del Prof. Baerends, alguns membres de l'IQC van utilitzar aquesta tècnica per reduir de forma dramàtica el cost de les integrals de solapament necessàries per fer càlculs de semblança (J. Mestres, M. Solà, M. Duran and R. Carbó. *On the calculation of ab initio quantum molecular similarities for large systems: Fitting the electron density.* **J. Comput. Chem. 15 (1994) 1113-1120**). Això va suposar un gran avenç en la teoria de la semblança molecular quàntica desenvolupada pel Dr. Ramon Carbó-Dorca a la nostra Universitat. Aquesta va ser una de les primeres influències destacades del treball del Prof. Baerends a l'IQC.

2. Desenvolupament juntament amb el Prof. Ziegler del primer mètode per fer càlculs d'estats excitats a nivell DFT a l'any 1976 basat en el fet que els estats excitats es poden representar com una combinació de determinants de Slater. Aquest va ser l'únic mètode pel càlcul dels estats excitats fins a l'arribada dels mètodes DFT depenent del temps a mitjans dels 90.

3. Entre els estudis dels efectes relativistes en els càlculs mecanoquàntics cal destacar la reinterpretació feta pel Prof. Baerends i col·laboradors sobre l'origen de la contracció relativista de la distància d'enllaç. El Prof. Baerends va demostrar que es tractava d'un efecte de la correcció del terme de massa-velocitat en l'energia cinètica.

4. En el camp dels estudis relativístics ha estat molt important l'aportació feta pel Prof. Baerends i col·laboradors de l'aproximació d'ordre zero (ZORA). Aquesta

aproximació ofereix una solució barata i molt eficient de les equacions de Dirac de dues components i es troba actualment implementada en la major part de programes estàndard de càlcul mecanoquàntic.

5. Realització d'estudis fonamentals que connecten la teoria DFT amb la correlació electrònica a través dels forats de correlació i bescanvi i de la densitat de correlació i bescanvi. Moltes de les idees desenvolupades pel Prof. Baerends en aquest camp han servit d'inspiració pel desenvolupament fet per membres de l'IQC dels índexs de localització i deslocalització i els indicadors d'aromaticitat (veure articles de revisió: J. Poater, M. Duran, M. Solà and B. Silvi. *Theoretical evaluation of electron delocalization in aromatic molecules by means of AIM and ELF topological approaches.* **Chem. Rev., 105 (2005) 3911-3947**; E. Matito, M. Solà, P. Salvador and M. Duran. *Electron Sharing Indexes at the Correlated Level. Application to Aromaticity Measures.* **Faraday Discuss., 135 (2007) 325-345** i E. Matito and M. Solà. *The role of electronic delocalization in transition metal complexes from the electron localization function and the quantum theory of atoms in molecules viewpoints.* **Coord. Chem. Rev., 253 (2009) 647-665**).

6. Determinació per primer cop en sistemes senzills del potencial de correlació-bescanvi exacte a partir d'una densitat exacta calculada amb un mètode full-CI. Això permet estudiar les propietats que ha de tenir el potencial de correlació-bescanvi exacte. També permet comprovar si la correlació o el bescanvi és més important per determinades reaccions, el que ha servit de base en alguns estudis fets per membres de l'IQC (M. Swart, M. Solà and F.M. Bickelhaupt. *Energy landscapes of nucleophilic substitution reactions: A comparison of density functional theory and coupled cluster methods.* **J. Comput. Chem., 28, (2007) 1551-1560**). Aquest tipus d'estudis iniciats pel Prof. Baerends són fonamentals pel disseny de nous funcionals. Les aportacions del Prof. Baerends en aquest camp han tingut especial incidència en la proposta recent d'un nou funcional feta per membres de l'IQCC (M. Swart, M. Solà and F. M. Bickelhaupt. *A new all-round density functional based on spin states and S_N2 barriers.* **J. Chem. Phys., 2009, 113 (2009) 9721–9726**).

7. Un resultat important de la recerca del Prof. Baerends és el reconeixement de la importància del decaïment Coulòmbic del potencial de Kohn-Sham per determinar propietats de resposta com les (hiper)polaritzabilitats. Això ha portat al Prof. Baerends a desenvolupar nous funcionals com ara el LB94, el SAOP o el GRAC. Aquests descobriments han tingut una incidència molt gran en la recerca de membres de l'IQC que treballen en el tema de les propietats òptiques no lineals (veure a tall d'exemple: M. Torrent-Sucarrat, M. Solà, M. Duran, J. M. Luis and B. Kirtman. *Basis Set and Electron Correlation Effects on Initial Convergence for Vibrational Nonlinear Optical Properties of Conjugated Organic Molecules.* **J. Chem. Phys., 120 (2004) 6346-6355**).

8. El Prof. Baerends ha derivat una prova del teorema de Koopman per les energies monoelectròniques Kohn-Sham. La connexió entre les energies monoelectròniques i el potencial d'ionització del sistema es demostra molt més precisa en la teoria DFT que en els càlculs Hartree-Fock. Aquest aspecte és important en la justificació de l'ús de la teoria d'orbitals moleculars (OM) Kohn-Sham com a mètode d'OM qualitatiu per estudiar l'enllaç químic.

9. Un dels aspectes més rellevants de la recerca del Prof. Baerends ha estat el desenvolupament d'eines per l'anàlisi de la naturalesa de l'enllaç químic, en particular, el seu esquema de descomposició de l'energia on la component d'energia d'interacció orbitalària es descomposa entre les diferents components de simetria. Aquest esquema de descomposició de l'energia ha aportat una comprensió molt detallada de l'enllaç químic, sobretot pel que fa a l'efecte de la interacció electrostàtica i els efectes cinètics. S'han publicat numeroses aplicacions d'aquest esquema, algunes d'elles fetes a l'IQCC (veure a tall d'exemple: M. Cases, G. Frenking, M. Duran and M. Solà. *Molecular Structure and Bond Characterization of the Fischer-Type Chromium-Carbene Complexes* $(CO)_5Cr=C(X)R$ *(X= H, OH,* OCH_3*,* NH_2*,* $NHCH_3$ *and R= H,* CH_3*,* $CH=CH_2$*, Ph,* $C\equiv CH$*).* **Organometallics, 21 (2002) 4182-4191** i F. Feixas, M. Solà and M. Swart. *Chemical bonding and aromaticity in metalloporphyrins.* **Can. J. Chem., 87 (2009) 1063-1073**).

10. A remarcar també entre els grans assoliments del Prof. Baerends, el desenvolupament i implementació d'un mètode molt acurat pel càlcul de l'estructura electrònica en sistemes periòdics en l'anomenat programa BAND. Aquest programa ha permès l'estudi detallat de les interaccions molècula-superfície i la investigació de processos molt importants com són la catàlisi heterogènia i la corrosió.

11. Implementació de la teoria DFT depenent del temps pel càlcul de les funcions resposta que ha permès el càlcul de nombroses propietats espectròscopiques de molècules grans amb una bona precisió. El Prof. Baerends i els seus col·laboradors han descobert l'error que presenta aquest mètode pel càlcul de les (hiper)polaritzabilitats en el cas de cadenes conjugades de mida molt gran (cas dels polímers). A més, s'ha aconseguit entendre els espectres visibles de porfirines amb els resultats obtinguts amb els nous funcionals. Aquests nous resultats donen suport a idees proposades als anys 50 per Gouterman.

12. Mitjançant estudis de dinàmica molecular Car-Parrinello, el Prof. Baerends i col·laboradors han permès determinar que en l'oxidació del peròxid d'hidrogen catalitzada per Fe^{+2} en solució aquosa (reacció Fenton) l'intermedi reactiu més important és el FeO^{2+} i no pas el radical OH· com s'havia postulat en la major part d'estudis previs. Aquest resultat connecta la reacció de Fenton amb la reactivitat de l'enzim P450.

13. En els darrers anys, el Prof. Baerends ha dedicat molts d'esforços a desenvolupar la teoria del funcional de la densitat matricial (DMFT) i també a la seva variant depenent del temps. Si bé els resultats preliminars són molt prometedors i podria ser en el futur el mètode habitual de càlcul, encara falta millorar-ne el desenvolupament i la implementació. Seguint aquesta línia hi està treballant actualment a l'IQCC el Dr. E. Matito (veure a tall d'exemple: X. López, F. Ruiperez, M. Piris, J. M. Matxain, E. Matito and J. M. Ugalde, *Performance of PNOF5 Natural Orbital Functional for Radical Formation Reactions: Hydrogen Atom Abstraction and C-C and O-O Homolytic Bond Cleavage in Selected Molecules.* **J. Chem. Theory Comput. 8 (2012) 2646-2652**).

4.b Projecció de mestratge

La llavor del Prof. Baerends

Una de les tasques més importants que ha dut a terme el Prof. Baerends ha estat la direcció o codirecció de 34 Tesis doctorals així com l'acolliment en el seu grup de molts postdocs que han

aprofitat l'estada a la Vrije Universiteit Amsterdam per incrementar els seus coneixements. La intensa tasca dinamitzadora en el camp de la química teòrica ha fet que a moltes universitats hi hagi deixebles directes seus (ex-estudiants de doctorat, postdocs i investigadors visitants).

Entre els seus deixebles, ex-estudiants de doctorat del Prof. Baerends, destaca la presència del **Prof. J. G. Snijders**, catedràtic a la Rijksuniversiteit Groningen des de l'any 1997 fins a la seva mort ocorreguda l'any 2003. Durant aquest període va ser el director de Tesi d'un dels membres de l'IQC, el Dr. Marcel Swart. El Prof. Snijders va fer contribucions molt significatives en el camp dels efectes relativistes i al desenvolupament de la DFT depenent del temps. Va publicar 122 articles que van rebre un total de 8627 cites. El seu índex h és de 43. També esmentar el **Prof. M. Nooijen** que és professor associat a la Universitat de Waterloo al Canadà i que ha treballat intensament sobre els mètodes coupled-cluster, acoblaments vibrònics i efectes relativistes. L'any 2003 va guanyar la prestigiosa medalla de la Internationcal Academy of Quantum Molecular Science. També cal mencionar el **Prof. F. M. Bickelhaupt** que actualment ocupa la càtedra que ha deixat vacant el Prof. Baerends. El Prof. Bickelhaupt està especialitzat en l'estudi de la naturalesa de l'enllaç químic i de la reactivitat química i ha rebut nombrosos premis de recerca com ara el Jonge Chemici award (NWO-CW) l'any 2001 o el VICI award (NWO) l'any 2002. També cal esmentar el nom del **Prof. R. Van Leeuwen**, catedràtic a la Universitat de Jyvaskyla a Finlàndia i que ha fet importants contribucions en el camp de la correlació electrònica i de la teoria DFT. Conjuntament amb el Prof. Baerends el Prof. Van Leeuwen va desenvolupar un dels nous funcionals (LB94). També cal parlar del **Prof. T. Ziegler**, catedràtic a la Universitat de Calgary (Canadà), i que ha fet grans contribucions a la química teòrica i computacional i al desenvolupament del programa ADF. El Prof. Ziegler ha publicat uns 500 articles que han rebut un total de 19333 cites i té un índex h de 67. És un dels grans químics canadencs actuals i va treballar a Amsterdam durant un període doctoral i també un de postdoctoral. Ha obtingut nombrosos premis de recerca: El Alcan Lecture Award (The Canadian Society of Chemistry) el 1994, el premi Pure and Applied Inorganic Chemistry (The Canadian Society of Chemistry) el 2000, el 2004 la prestigiosa Schrödinger Medal, World Association for Theoretically Oriented Chemists (WATOC) i el 2005 el Steacie Award (The Canadian Society of Chemistry). Al llarg de 2009 la revista *Canadian Journal of Chemistry* ha dedicat dos volums al Prof. Ziegler, i en un d'ells hi ha un article de membres de l'IQC (F. Feixas, M. Solà and M. Swart. *Chemical bonding and aromaticity in metalloporphyrins.* **Can. J. Chem., 87 (2009) 1063-1073**). Cal afegir a aquesta llista el **Dr. O. V. Gritsenko** que ha treballat durant més de 20 anys amb el Prof. Baerends i s'ha guanyat una gran reputació en el camp de la teoria del funcional de la densitat i la seva versió depenent del temps. Actualment és investigador permanent a la Vrije Universiteit Amsterdam. Finalment mencionar el treball dels **Drs. E. van Lenthe**, **G. Te Velde** i **S. J. A. van Gisbergen**, tots els ex-estudiants de doctorat del Prof. Baerends, que han fets contribucions molt importants i que han treballat intensament en la implementació de molts mètodes en el programa ADF.

Entre els visitants de la Universitat de Girona que han rebut les ensenyances del Prof. Baerends, hem de mencionar les visites del **Dr. Miquel Solà** (actualment catedràtic d'universitat de la UdG) els anys 1994, 2005, 2007 i 2009, l'estada postdoctoral de tres anys (2004-2007) i altres visites curtes anteriors com a estudiant de doctorat (3 mesos el 2001, 1 mes el 2002) i també posteriors (3 mesos el 2013) del **Dr. Jordi Poater** actualment investigador contractat a l'IQCC, les estades del **Dr. Marcel Swart** (actualment investigador ICREA sénior a l'IQCC) com a postdoc primer al grup de Prof. Baerends des de 2004 a 2006 i els anys 2007 i 2009, la visita d'un mes del **Dr. Pedro Salvador** (actualment professor agregat de la UdG) l'any 2006, la visita d'un mes del **Dr. Sergei Vyboishchikov** (actualment professor agregat de la UdG) l'any 2009 i les estades d'estudiants de doctorat com ara en **David Hugas** l'any 2008, l'**Anna Dachs** l'any

2009, **Laia Guillaumes** (2 mesos el 2012 i 3 mesos el 2013). Finalment la **Dra. Sílvia Simon** el mes de juliol de 2013 va fer una visita d'un setmana. Tots ells han rebut directament la influència del Prof. Baerends a través del seu mestratge.

Foto 1. Tribunal de la Tesi del Dr. G. T. de Jong celebrat a Amsterdam el 24 d'abril de 2007 amb presència del Prof. E. J. Baerends i del Dr. M. Solà.

El reconeixement al Prof. Baerends

Dos fets són especialment rellevants per al reconeixement de l'autoritat acadèmica del candidat. En primer lloc, l'organització d'un simposi internacional en el seu honor ("Evert Jan Baerends Symposium on the Occasion of his Sixtieth Birthday") que va tenir lloc el 4 de novembre de 2005 a Amsterdam, i on investigadors europeus i americans es van juntar per fer-li reconeixement i presentar les seves darreres investigacions. Precisament a aquesta reunió va assistir com a ponent invitat un membre de l'IQCC (Dr. Solà). En segon lloc, el seu recent fitxatge com a professor invitat de gran prestigi (World Class University Distinguished Professorship) a la Universitat de Ciència i Tecnologia de Pohang a Corea del Sud.

El servei del Prof. Baerends a la Societat

El candidat ha estat durant varis anys el Coordinador de l'Àrea de Química de la National Science Foundation d'Holanda (NWO), la principal agència per la recerca en Química a Holanda amb un pressupost anual de 20 milions d'euros. També ha estat membre del comitè per la Recerca Fonamental en Física d'Holanda amb un pressupost de 100 milions d'euros. Ha participat en el comitè de creació de l'Institut de Química de Leyden i és el coordinador de l'Escola de Recerca Holandesa de Química Molecular. Finalment ha participat de forma regular en comissions per avaluar projectes europeus.

Foto 2. Evert Jan Baerends Symposium on the Occasion of his Sixtieth Birthday celebrat a Amsterdam el 4 de novembre de 2005.

4.c Relació amb la UdG:

La relació del Prof. Baerends amb la Universitat de Girona és llarga i intensa. Es va iniciar el febrer del 1994 amb la visita de 11 setmanes del Dr. Solà al seu grup de recerca. A partir d'aquí les anades i vingudes des de la Universitat de Girona a la Vrije Universiteit i a la inversa s'han succeït i han donat com a fruit un gran nombre de publicacions conjuntes, així com la signatura de varis convenis. El primer d'aquests convenis es titula "*Framework Collaboration Agreement Between The Vrije Universiteit Amsterdam and The University of Girona Related to the Euromediterranean International Campus On Tourism Sustainability and Water (E-MTA)*". 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. El 24 de gener del 2013 es va produir la primera reunió del Comitè de Seguiment del conveni signat per les dues Universitats. En aquesta reunió es va acordar el model de conveni per les tesis cotutelades entre les Universitats de Girona I Vrije Amsterdam. Hi ha dos estudiants (Laia Guillaumes i Juan Pablo Martínez) que ja han enviat el seu conveni a signar i que faran una tesi cotutelada entre les Universitats de Girona i la Vrije Amsterdam.

De les visites de membres del grup de recerca del Prof. Baerends a Girona destaquem:

- Tres visites del mateix Prof. Baerends els anys 1996, 2008 i 2010 cadascuna d'elles d'una setmana de duració. El 2008 va participar com a conferenciant en el VIII Girona Seminar i el 2010 en el IX Girona Seminar, tots ells organitzats per l'IQCC.
- Onze visites del Prof. Dr. F. Matthias Bickelhaupt des de l'any 1997 fins el 2009 amb durades variables d'un mínim de 2 setmanes i un màxim de 3 mesos. Ha participat com a conferenciant en els VII, VIII, IX Girona Seminars i està previst que participi en el XI Girona Seminar.
- Dues visites de la Dr. Celia Fonseca Guerra els anys 1998 i 2001 de tres mesos de duració. El 2012 va participar com a conferenciant en el X Girona Seminar.

- Una visita l'any 2006 de dos mesos de l'estudiant de doctorat Ruud Visser.
- Dues visites de dos mesos del Dr. Marcel Swart a l'IQC quan era postdoc al grup del Prof. Baerends els anys 2004 i 2005.

Foto 3. Primera visita del Prof. Evert Jan Baerends a Girona el 19 de juliol de 1996.

Un aspecte destacable de la seva relació amb membres de la UdG és que el Prof. Baerends va aportar una carta de referència en el procés que va conduir al Dr. Marcel Swart a l'Institut de Química Computacional, primer com ICREA-Júnior i aquest mateix 2009 com ICREA-Sènior. També va ser decisiva la seva carta de suport per la concessió de la Distinció de la Generalitat de Catalunya per a la Promoció de la Recerca Universitària 2001 al Dr. Miquel Solà de l'Institut de Química Computacional i Catàlisi.

Foto 4. El Prof. Evert Jan Baerends al VIII Girona Seminar el 10 de juliol de 2008.

De les visites de membres dels grup de recerca de l'Institut de Química Computacional i Catàlisi (IQCC) de la Universitat de Girona destaquem:

- Quatre visites del Dr. Miquel Solà els anys 1994, 2005, 2007 i 2009 cadascuna d'elles amb una duració d'entre una i onze setmanes.
- Dues visites com a estudiant de doctorat del Dr. Jordi Poater, 3 mesos el 2001 i 1 mes el 2002.
- Una estada postdoctoral de tres anys (2004-2007) del Dr. Jordi Poater actualment contractat a l'IQCC.
- Una visita de tres mesos (2013) del Dr. Jordi Poater actualment contractat a l'IQCC.
- Una visita d'un mes del Dr. Pedro Salvador l'any 2006.
- Dues visites de dues setmanes de duració del Dr. Marcel Swart com a investigador ICREA júnior de l'IQC els anys 2007 i 2009.
- Una visita de tres mesos del estudiant de doctorat David Hugas l'any 2008.
- Una visita d'un mes del Dr. Sergei Vyboishchikov l'any 2009.
- Una visita de tres mesos de duració de l'estudiant de doctorat Anna Dachs l'any 2009.
- Una visita de dos mesos de duració de l'estudiant de doctorat Laia Guillaumes l'any 2012.
- Una visita de tres mesos de duració de l'estudiant de doctorat Laia Guillaumes l'any 2013.
- Una visita d'una setmana de la Dra. Sílvia Simon el juliol del 2013.

Fruit d'aquesta intensa relació, el grup del Prof. Baerends té uns 35 articles internacionals publicats conjuntament amb les persones de la UdG esmentades. A més, en molts de congressos i reunions de caire internacional s'hi han presentat ponències, comunicacions orals i pòsters amb autoria de membres del grup del Prof. Baerends i alguna de les persones de la UdG relacionades. Finalment convé destacar el fet que dos membres actuals de l'IQCC (Drs. Swart i Solà) són co-autors del programa Amsterdam Density Functional (ADF) del qual el Prof. Baerends n'és l'autor principal.

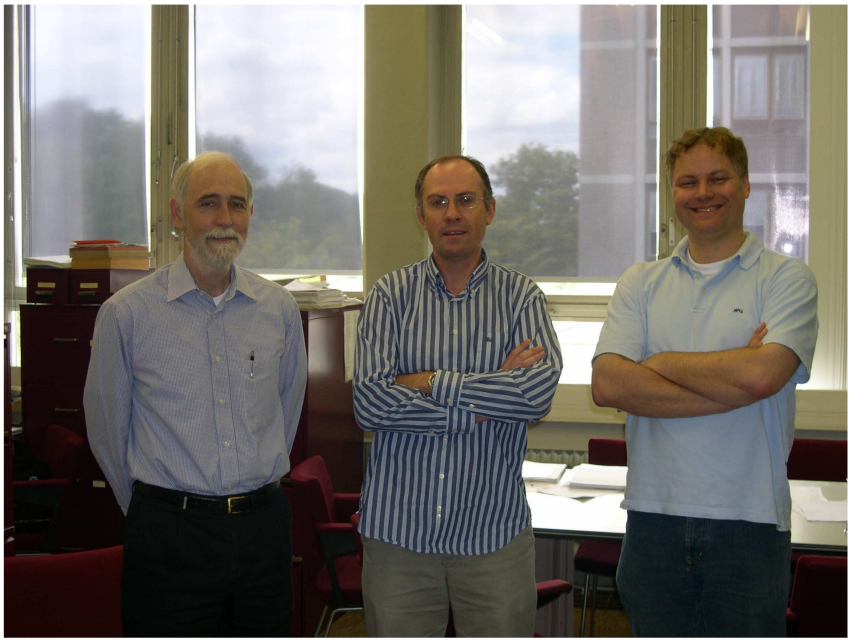

Foto 5. Al despatx del Prof. Evert Jan Baerends el 15 de juny de 2009.

El Prof. Baerends té una projecció molt important, doncs, de mestratge sobre varis professors i investigadors dels actuals Departament de Química i 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 Profs. Vicenç Branchadell i Mariona Sodupe de la Universitat Autònoma de Barcelona, amb el Prof. Josep Maria Poblet de la Universitat Rovira i Virgili i amb el Prof. Carles Bo de l'Institut Català d'Investigacions Químiques.

Foto 6. El Prof. Evert Jan Baerends amb el Dr. Marcel Swart al Congrés DFT2007 el 26 d'agost de 2007 a Amsterdam .

<u>El grup de recerca del Prof. Baerends ha publicat 50 articles internacionals conjuntament amb diversos membres i ex-membres de l'Institut de Química Computacional i Catàlisi:</u>

Miquel Duran
Miquel Solà
Sílvia Simon
Marcel Swart
Jordi Poater
Eduard Matito
David Hugas
Sílvia Osuna

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Chem. Eur. J., 19 (2013) 7416-7422.

Aquests articles han rebut un total de 1000 cites (h = 17) i tres d'ells han estat considerats "*hot papers*" per l'Essential Science Indicators.

Llistat de publicacions del Prof. Baerends amb altres membres de la comunitat científica catalana:

E. J. Baerends, V. Branchadell and M. Sodupe.
Atomic Reference Energies for DFT calculations
Chem. Phys. Lett. 265 (1997) 481-489.

M. Sodupe, J. Bertran, L. Rodríguez-Santiago and E. J. Baerends.
The ground state of the $(H_2O)_2^+$ radical cation. DFT versus post-Hartree-Fock methods.
J. Phys. Chem. A, 103 (1999) 166-170.

J. A. Fernández, X. López, C. Bo, C. de Graaf, E. J. Baerends and J. Poblet.
Polyoxometalates with internal cavities: redox activity, basicity and cation encapsulation in $[X^{n+}P\text{-}5W\text{-}30O\text{-}110]^{(15-n)-}$ Preyssler complexes, with $X=Na^+$, Ca^{2+}, Y^{3+}, La^{3+}, Ce^{3+} and Th^{4+}.
J. Am. Chem. Soc. 128 (2007) 12244-12253.

4.d Curriculum Vitae complet (en anglès)

CURRICULUM VITAE E. J. BAERENDS

Name: Evert Jan Baerends

Home: Militairenweg 15, 2051 ET Overveen, The Netherlands
tel. +31 23 5274310

Work: Dep. of Chemistry and Pharmaceutical Sciences,
Faculty of Exact Sciences (FEW), VU University,
De Boelelaan 1083, 1081 HV Amsterdam, The Netherlands
tel. +31 20 59 87 623; emeritus as of September 2010

World Class University professor at
Pohang University of Science and Technology, Dep. of Chemistry
San 31, Hyojadong, Namgu
Pohang 790-784, South-Korea
tel. +82-54-279-5230; secr. +82-54-279-8133; fax +82-54-279-8137

Adjunct Professor at Department of Chemistry,
King Abdul Aziz University, Jeddah 21589, Saudi Arabia

Date/place of birth: 17 september 1945, Voorst, The Netherlands
Marital status: Married, two children
Citizenship: Dutch

Education: 1957-1963 Gymnasium β, Christelijk Lyceum "Oostergo", Dokkum
1963-1967 Kandidaatsstudie Scheikunde Vrije Universiteit (cum laude) (Bachelor Chemistry)
1967-1970 Doktoraalstudie Fysische Chemie Vrije Universiteit (cum laude) (Master with major Physical Chemistry)
Dec. 1970 – Feb. 1975: Ph. D. work, supervisor Prof. Dr. Ir. P. Ros
Thesis: "Self-Consistent Molecular Hartree-Fock-Slater calculations"

Work Experience: 1975-1976: Postdoctoral Fellow at the Vrije Universiteit, Amsterdam

1976-1981: Lecturer in History and Philosophy ("Encyclopedia") of Chemistry at the Vrije Universiteit

1981-2010: Professor of Theoretical Chemistry at the Vrije Universiteit; 2010- .. Emeritus professor at VU university

2008-2013: World Class University professorship at Pohang University of Science and Technology, Pohang, South-Korea

2011- .. Adjunct Professor at King Abdul Aziz University, Department of Chemistry, Jeddah, Saudi Arabia

Teaching Experience: 1970-1975: Assistence at Laboratory Courses (Inorganic/Physical Chemistry)

1976-1981: First-year lectures "Encyclopedia of Chemistry"

1977-present: Several Courses, regularly:

Second-year lectures Chemical Bonding / Theoretical Chemistry

Third-year course Group Theory

Third-year course Theoretical Chemistry

Graduate Course Theoretical Chemistry

Graduate Course: Theory, Computation and Spectroscopy (in Master-program Physical Sciences, jointly with University of Amsterdam)

Awards etc. Unilever student award, 1970

Koninklijke/Shell Price, 1976

Member of the International Academy of Quantum Molecular Science, July 1999

Recipient of Schlumberger Medal, June 20, 2001, Cambridge, UK

Membership Royal Netherlands Academy of Science, 2004

World Class University Distinguished Professorship at Pohang University of Science and Technology, Pohang, South-Korea, 2008- 2013

2010 Schrödinger Medal of the World Association of Theoretically Oriented Chemists (WATOC)

Citations / Impact ca. 420 publications, H-index: 81

Total nr of citations: over 37 000; average per article: 87

Listed at ISI Web of Science's website http://isihighlycited.com/

of the world's most cited authors of the past 25 years

Listed at the Royal Society of Chemistry's website

http://www.rsc.org/chemistryworld/News/2007/April/23040701.asp

of the most cited living chemists, ranked according to H-index (highest Dutch chemist on the list)

Listed among top-100 most cited chemists (over previous 10 years): Nov. 2005, Nov. 2006, Nov. 2007 (listing was discontinued)

Visiting professorships

Visiting professorship at Universität Konstanz, Germany, 1988

Grant from Deutsche Akademische Austauschdienst (DAAD) for visit to Universität-Gesamthochschule Siegen, Germany, 1986

Visiting professorship at Università Basilicata, Potenza, Italy, 1990

Visiting professor in Switzerland (Geneva, Lausanne, Fribourg) for lectures in the Convention Intercantonale Romande pour l'Enseignement du 3e Cycle en Chimie, sept. 1993

Visiting professor at the University of Fribourg, Switzerland, 95/96

Iberdrola Foundation visiting professor at Universita Autonoma de Barcelona, june-august 1996

Visiting professor at Universita Autonoma de Barcelona, july 1997 and july 1998.

Visiting professor at university of Auckland, New Zealand, april 1998

Schlumberger Professor at Cambridge University, UK, 2001, 2002, 2003;

Visiting professor in Switzerland (Geneva, Lausanne, Fribourg) for lectures in the Convention Intercantonale Romande pour l'Enseignement du 3e Cycle en Chimie, Nov. 2002

Visiting professor at Université Pierre et Marie Curie, Paris, France, 2005

Editorial Boards:

Advisory Editorial Board Theoretical Chemistry Accounts, 1997-

Advisory Editorial Board Physical Chemistry and Chemical Physics, 1998-2001

Advisory Editorial Board, Chemical Physics Letters, 2001 -

Advisory Editorial Board PhysChemComm 2002 – 2003

Member Editorial Board Journal of Computational Chemistry 2004-

Editorial board Research Letters in Physical Chemistry 2009-

Selection of administrative positions:

1982-1985 Chairman Dep. of Inorganic and Theoretical Chemistry

1983-1886 Secretary of the section for Quantumtheoretical Chemistry (QTC) of the Netherlands Foundation for Research (NWO)

1985-1989 Chairman Dep. of Physical and Theoretical Chemistry

1986-1989 Chairman of section for Quamtumtheoretical Chemistry (QTC) of the Netherlands Foundation for Research (NWO)

1990-1993 Dean of the Faculty of Chemistry

1992-1997 Member of the Management Committee of the COST Action D3 of the EU "Reactivity, Dynamics and Chemical Reactions; Simulation, Modeling and Experiment"

1992-1998 Member of the Steering Committee of the European Science Foundation programme for Relativistic Effects in Heavy Elements (REHE)

1993 Chairman first REHE conference, June '93, De Haan, Belgium.

1994-1996 Member of the Research Committee of the Holland Research School of Molecular Chemistry (HRSMC)

1995-1996 Chairman of the section for Quamtumtheoretical Chemistry (QTC) of the NWO Foundation for Chemical Research (SON-NWO)

1996-1998 Member of the Board of the Research School HRSMC

1998-2009 Chairman of the Board of the Research School HRSMC

1997-2002 Chairman of the Committee WGS of the NWO Foundation for National Computing Facilities NCF, and advisory member of the board of NCF

2002-2009 Member of the WGS committee of NCF

1997-2000 Chairman of the section Spectroscopy and Theory of the NWO Foundation for Chemical Research (CW-NWO).

1997-2002 Member of the Management Committee of the COST Action D9 of the EU "Computational Physics and Chemistry of Increasingly Complex Systems"

1998-2000 Chairman Beleidsadviescommissie Fysische Chemie of CW-NWO

1998-2000 Chairman Selection Committee for the National Supercomputer of NCF-NWO

2001-2010 Member of the Board, FOM

2002-2005 Member of the Board, Faculty of Exact Sciences Vrije Universiteit

2004-2010 Member of the Board, Division of Chemistry, NWO
2006-2008 Vice-chairman, 2008 - 2010 Chairman

2004- Member Supervisory Board Leyden Department of Chemistry

2005 Evaluator for the Academy of Finland Programme of Centres of Excellence in Research 2006-2011

2006-2011 Co-chair Scientific Advisory Board of the Finnish Centre of Excellence in Computational Molecular Science

2006-2007 Member Selection Committee National Supercomputer

2007 Chairman of the Conference “Applications of Density Functional Theory”, Amsterdam, August 26-30, 2007 (410 participants)

2008-2009 Secretary of the Section Chemistry of the Royal Netherlands Academy of Science

2008-2009 Member of the Advisory Committee for Technical Sciences, Mathematics, Informatics, Physics and Chemistry of the Royal Netherlands Academy of Science

2008-2013 World Class University Distinguished Professorship at Pohang University of Science and Technology, Pohang, South-Korea

2011 Scientific Committee of the VIIth congress of the International Society for Theoretical chemical Physics, Tokyo, Japan, Sept. 2011

2010- Member of the Board of the World Association of Theoretical and Computational Chemists (WATOC)

RESEARCH

A) Summary of research interests.

1) Many-electron theory, in particular the density functional theory (DFT) for many-electron systems.

2) Development and implementation of new computational techniques, mostly based on density functional theory: the Amsterdam Density Functional (ADF) and BAND program systems.

3) Understanding, explaining and predicting properties of molecules and (transition-metal) complexes from their electronic structure. Energy decomposition methods for interactions between molecular fragments, and between molecules and infinite two-dimensional systems (metallic surfaces). Studies of structure, bonding and reactivity (catalysis), including *ab initio* molecular dynamics (Car-Parrinello or AIMD) study of reactivity in solution.

4) Development of time-dependent DFT and application to response properties such as (hyper)polarizabilities, Raman intensities, electronic excitation spectra, electronic and vibrational circular dichroism.

5) Relativistic effects in the chemistry and spectroscopy of heavy element compounds.

6) Surface-molecule interactions: scattering from and dissociation at metallic surfaces of small molecules.

7) Density *matrix* functional theory.

B) Summary of results.

The main result of the research has been theoretical elucidation and further development of density functional theory (DFT), and more recently density matrix functional theory (DMFT). DFT has been used to develop and and implement computational methods exploiting the advantages this theory offers for speeding up actual electronic structure calculations. Applications in diverse fields have been made.

1) An important early result of the research has been the development in the early seventies of the now universally employed methodology for DFT calculations, using a combination of three ingredients: a) the conventional expansion method of quantum chemistry ("basis sets") for the Kohn-Sham orbitals; b) the use of auxiliary functions (called "density fitting," or "resolution of the identity") for the Coulomb potential evaluation, in order to make the calculations N^3 scaling; c) 3D numerical integration for calculation of (parts of) the Hamiltonian matrix elements. A comprehensive program system, called ADF, has been developed over the years. It is capable of handling large systems such as transition-metal complexes and clusters, large organic systems (several base pairs of DNA), periodic systems (3-, 2- or 1-dimensional) and heavy element compounds (relativistic effects).

2) Relativistic effects have been first (late seventies and eighties) addressed by perturbation theory (in a "coupled" form) (thesis work of J. G. Snijders), later (nineties) by a two-component regular hamiltonian, i.e. the in-house developed and now much applied zero-order regular approximation (ZORA) (thesis work of E.

van Lenthe). Amongst the studies of relativistic effects, an early important result has been the “Dutch revolution” of reinterpretation of the origin of the relativistic contraction of bond lengths.

3) Fundamental studies of the connection between the DFT approach to electron correlation and the traditional insights based on density matrices have enabled the expression of the key quantities of DFT (exchange-correlation energy density and Kohn-Sham one-electron potential) in terms of wavefunction derived quantites, notably the conditional amplitude. This has for example led to new functionals for the Kohn-Sham potential, improving greatly response property calculations, and to the derivation in DFT of the analogue of Koopmans’ theorem for one-electron energies. This theorem, establishing the connection between one-electron energies and ionization energies, is well known in Hartree-Fock theory, This connection has always been denied in DFT, but proves to hold much more accurately in DFT than in Hartree-Fock theory. This is very important for the use of Kohn-Sham MO theory as a qualitative MO method in chemistry.

4) Development of bond energy analysis tools and concepts, notably in the context of Kohn-Sham MO theory, which establishes the Kohn-Sham MO theory as a full fledged chemical theory for structure and bonding. Many applications to chemically interesting systems and problems.

5) The development and implementation in the eighties of a highly accurate method for electronic structure calculations on periodic systems, has proven to be extremely useful for the generation of very reliable potential energy surfaces for surface-molecule interaction. A breakthrough in the theoretical modelling of surface-molecule interactions, which is very important for reactivity at surfaces (heterogeneous catalysis, corrosion) has occurred by the performance of dynamics calculations (by the collaboration with G. J. Kroes) on these very accurate potential energy surfaces, yielding a complete description of all scattering and dissociation channels.

6) Implementation of time-dependent DFT based response methods, in combination with functional development based on theoretical work (see 3) have enabled the calculation of many spectroscopic properties of (large) molecules, with very gratifying accuracy.

7. Solvent effects on reactivity at a transition-metal center are being studied with Car-Parrinello molecular dynamics, which reveal in a striking manner the importance of the H-bond networks in water for reaction mechanisms.

8) In recent years we have been developing methods based on density *matrix* functional theory. In principle this theory affords a more transparent treatment of electron correlation in terms of Fermi and Coulomb holes which can be expanded with the help of the natural orbitals. Linear response based methods are being developed to obtain excitation energies and polarizabilities.

Publication List E.J. Baerends

1. E.J. Baerends, D.E. Ellis, P. Ros
"A theoretical Study of the Interaction of Ethylene with Transition Metal Complexes"
Theoret. Chim. Acta, 27 (1972) 339-354.

2. E.J. Baerends, D.E. Ellis, P. Ros
"Self-consistent molecular Hartree-Fock-Slater calculations. I. The computational procedure"
Chem. Phys. 2 (1973) 41-51.

3. E.J. Baerends, P. Ros
"Self-consistent molecular Hartree-Fock-Slater calculations. II. The effect of exchange scaling in some small molecules"
Chem. Phys. 2 (1973) 52-59.

4. E.J. Baerends, P. Ros
"Level ordering in Ferrocene. A comparison between the Hartree-Fock-Slater and Hartree-Fock models"
Chem. Phys. Lett. 23 (1973) 391-393.

5. E.J. Baerends, P. Ros
"Self-consistent molecular Hartree-Fock-Slater calculations. III. The influence of non-spherical contributions to the electron density and potentials"
Chem. Phys. 8 (1975) 412-418.

6. E.J. Baerends, Ch. Oudshoorn. A. Oskam
"Photoelectron spectra and Xα calculations of iron pentacarbonyl and ethyleneiron tetracarbonyl"
Journ. Electr. Spectrosc. and Rel. Phenomena, 6 (1975) 259-267.

7. E.J. Baerends, P. Ros
"Hartree-Fock-Slater calculations on the charge distribution and ligand 1s binding energy shifts in carbonyl complexes"
Journ. Electr. Spectrosc. and Rel. Phenomena, 7 (1975) 69-74.

8. "Self-consistent molecular Hartree-Fock-Slater calculations"
Dissertatie, Vrije Universiteit, Amsterdam, 1975.

9. G. de With, D. Feil, E.J. Baerends
"Charge distribution in the nitrate ion"
Chem. Phys. Lett. 34 (1975) 497-499.

10. E.J. Baerends, P. Ros
"The electronic structure of transition metal carbonyl complexes. A comparison of Hartree-Fock-Slater calculations with UV photoelectron spectra and IR and Raman data"
Mol. Phys. 30 (1975) 1735-1747.

11. W. Heijser, A.Th. Kessel, E.J. Baerends

"Self-consistent molecular Hartree-Fock-Slater calculations. IV. On electron densities, spectroscopic constants and proton affinities of some small molecules"
Chem. Phys. 16 (1976) 371-379.

12. T. Ziegler, A. Rauk, E.J. Baerends
"The electronic structure of tetrahedral oxo-complexes. The nature of the "charge transfer" transitions"
Chem. Phys. 16 (1976) 209-217.

13. T. Ziegler, A. Rauk, E.J. Baerends
"On the calculation of multiplet energies by the Hartree-Fock-Slater method"
Theoret. Chim. Acta 43 (1977) 261-271.

14. J.G. Snijders, E.J. Baerends
"A non-parametrized pseudopotential scheme adapted to the Hartree-Fock-Slater model"
Mol. Phys. 33 (1977) 1651-1662.

15. D.E. Ellis, E.J. Baerends, H. Adachi, F.W. Averill
"Molecular cluster theory of CO chemisorption on a Nickel (100) surface"
Surface Science 64 (1977) 649-667.

16. A. Seth, E.J. Baerends
"H-bond contribution to the Compton profile of water"
Chem. Phys. Lett. 52 (1977) 248-251.

17. D.J. Miller, D. Haneman, E.J. Baerends, P. Ros
"Comparison of charge densities and pseudo charge densities for Si_2"
Phys. Rev. Lett. 41 (1978) 197-200.

18. D.E. Ellis, E.J. Baerends, H. Adachi, F.W. Averill
"Molecular cluster theory of CO chemisorption on a Nickel (100) surface"
Selected papers in Physics (Physical Society of Japan), 198 (Surface Physics) (1978) 96-114.

19. E.J. Baerends, P. Ros
"Evaluation of the LCAO Hartree-Fock-Slater method: Applications to transition-metal complexes"
Int. Journ. Quant. Chem. S12 (1978) 169-190.

20. J.G. Snijders, E.J. Baerends
"A perturbation theory approach to relativistic calculations. I. Atoms"
Mol. Phys. 36 (1978) 1789-1804.

21. A. Rosén, E.J. Baerends, D.E. Ellis
"Molecular cluster calculations for interpretation of CO chemisorption on a Ni (100) surface"
Surface Science 82 (1979) 139-164.

22. A. Seth, E.J. Baerends
"Compton profiles of aqueous solution of LiCl"
Chem. Phys. Lett. 64 (1979) 165-169.

23. C. Gooijer, E.J. Baerends, W. Oosterbeek
"Line broadenings within the alkali metal hyperfine multiplets of ion pairs and triple ions"
Journ. Chem. Soc. Faraday Transact II, 75 (1979) 1423-1427.

24. J.G. Snijders, E.J. Baerends, P. Ros
"A perturbation theory approach to relativistic calculations. II. Molecules"
Mol. Phys. 38 (1979) 1909-1929.

25. W. Heijser, E.J. Baerends, P. Ros
"Basis-set effects in the quantum mechanical description of transition-metal complexes"
J. Molec. Struct. 63 (1980) 109-120.

26. P.J.M. Geurts, J.W. Gosselink, A. van der Avoird, E.J. Baerends, J.G. Snijders
"Hartree-Fock-Slater-LCAO calculations on $[Fe_4S_4(SH)_4]^{0,2-,3-}$: a model for the 4-Fe active site in high potential iron protein and ferredoxin"
Chem. Phys. 46 (1980) 133-148.

27. T. Ziegler, J.G. Snijders, E.J. Baerends
"On the origin of the relativistic bond contraction"
Chem. Phys. Lett. 75 (1980) 1-4.

28. W. Heijser, E.J. Baerends, P. Ros
"Electronic structure of binuclear metal carbonyl complexes"
Faraday Symp. 14 (1980) 211-234.

29. T. Ziegler, J.G. Snijders, E.J. Baerends
"Relativistic effects on bonding"
Int. J. Quant. Chem. S14 (1980) 393.

30. C. Famiglietti, E.J. Baerends
"An LCAO-HFS investigation of the electronic structure of cobaltocene"
Chem. Phys. 62 (1981) 407.

31. T. Ziegler, J.G. Snijders, E.J. Baerends
"Relativistic effects on bonding"
J. Chem. Phys. 74 (1981) 1271-1284.

32. P. Pyykkö, J.G. Snijders, E.J. Baerends
"On the effect of d orbitals on relativistic bond-length contractions"
Chem. Phys. Lett. 83 (1981) 432.

33. D. Post, E.J. Baerends
"Cluster studies of CO adsorption. I. CO on small Li clusters"
Surface Science 109 (1981) 167.

34. J.G. Snijders, P. Vernooijs, E.J. Baerends
"Roothaan-Hartree-Fock-Slater atomic wave functions. Single-zeta, double-zeta, and extended slater-type basis sets for $_{87}Fr$-$_{103}Lr$"
Atomic data and nuclear data tables 26 (1981) 483.

35. E.J. Baerends, D. Post
"Analysis of CO-metal cluster interaction energies by the Hartree-Fock-Slater method"
in: Quantum theory of chemical reactions III (1982) 14,
Eds. R. Daudel, A. Pullman, L. Salem, A. Veillard, D. Reidel Publishing Comp.

36. D. Post, E.J. Baerends
"On the Hartree-Fock and Xα descriptions of small copper cluster electronic structures"
Chem. Phys. Lett. 86 (1982) 176.

37. D. Post, E.J. Baerends
"Cluster studies of CO adsorption. II. CO on small Al clusters"
Surface Science 116 (1982) 177.

38. L. Noodleman, D. Post, E.J. Baerends
"Symmetry breaking and ionization from symmetry equivalent inner shells and lone pairs in Xα theory"
Chem. Phys. 64 (1982) 159.

39. G. Jonkers, C.A. de Lange, L. Noodleman, E.J. Baerends
"Broken symmetry effects in the He(I) valence photoelectron spectrum of $Se(CN)_2$"
Mol. Phys. 46 (1982) 609.

40. J.G. Snijders, E.J. Baerends
"The influence of relativity on molecular properties: A review of the relativistic Hartree-Fock-Slater method"
in: Electron distribution and the chemical bond (1982) 111
Eds. M.B. Hall, P. Coppens, Plenum Publ. Corp.

41. B. Delley, D.E. Ellis, A.J. Freeman, E.J. Baerends, D. Post
"Binding energy and electronic structure of small copper particles"
Phys. Review B27 (1983) 2132.

42. D. Post, E.J. Baerends
"Cluster studies of CO adsorption. III. CO on small Cu clusters"
J. Chem. Phys. 78 (1983) 5663.

43. J.G. Snijders, W.J. van der Meer, E.J. Baerends, C.A. de Lange
"Hartree-Fock and Hartree-Fock-Slater electric field gradients H_2,CH_4) and their symmetry derivatives (CH_4)"
J. Chem. Phys. 79 (1983) 2970.

44. R.L. De Kock, E.J. Baerends, A. Oskam
"Fe-Fe π Bonding in $Fe_2(CO)_6S_2$?"
Inorg. Chem. 22 (1983) 4158.

45. R.L. DeKock, E.J. Baerends, P.M. Boerrigter, J.G. Snijders
"On the nature of the first excited states of the uranyl ion"
Chem. Phys. Lett. 105 (1984) 308.

46. G. Jonkers, W.J. van der Meer, C.A. de Lange, E.J. Baerends, J. Stapersma, G.W. KLumpp
"A UV photoelectron spectroscopic and Hartree-Fock-Slater MO-LCAO study of tetracyclo[3.3.0.0^{2,4}.0^{2,4}.0^{3,6}]oct-7-ene and related strained compounds"
J. Amer. Chem. Soc. 106 (1984) 587.

47. Th.A. van der Knaap, Th.C. Klebach, F. Visser, F. Bickelhaupt, P. Ros, E.J. Baerends, C.H. Stam, M. Konijn
"Synthesis and structure of aryl-substituted phospha-alkenes"
Tetrahedron **40** (1984) 765.

** Th.A. van der Knaap, F. Bickelhaupt, J. G. Kraaykamp, G. van Koten, J. P. C. Bernards, H. T. Edzes, W. S. Veeman, E. de Boer, E.J. Baerends
"η^1- and η^2-coordination in a (phosphaalkene)platimum(0) complex"
Organometallics **3** (1984) 1804-1811.

48. Roger L. DeKock, Evert Jan Baerends, Rudy Hengelmolen
"The nature of the LUMO in $Fe_2(CO)_6S_2$ and the bonding in $Fe_2(CO)_6S_2^{2-}$"
Organometallics 3 (1984) 289.

49. A. Rozendaal, E.J. Baerends
"Electron momentum density distribution in homonuclear diatomic molecules"
Chem. Phys. 87 (1984) 263.

50. Louis Noodleman, E.J. Baerends
"Electronic structure, magnetic properties, ESR, and optical spectra for 2-Fe Ferredoxin models by LCAO-Xs valence bond theory"
J. Amer. Chem. Soc. 106 (1984) 2316.

51. Roger L. DeKock, Evert Jan Baerends, Paul M. Boerrigter, Rudy Hengelmolen
"Electronic structure and bonding of $Hg(CH_3)_2$, $Hg(CN)_2$, $Hg(CH_3)(CN)$, $Hg(CCCH_3)_2$, and $Au(PMe)_3(CH_3)$"
J. Amer. Chem. Soc. 106 (1984) 3387.

52. W. Ravenek, E.J. Baerends
"The calculation of interaction energies using the pseudopotential Hartree-Fock-Slater-LCAO method"
J. Chem. Phys. 81 (1984) 865.

53. E.J. Baerends, J.G. Snijders, C.A. de Lange, G. Jonkers
"Application of the Hartree-Fock-Slater method in photoelectron spectroscopy"
in: Local density approximations in quantum chemistry and solid state physics,
Eds. J.P. Dahl, J. Avery, Plenum Press, New York, 1984, pp. 415.

54. A. Rozendaal, E.J. Baerends
"A momentum-space view of the chemical bond. The first-row homonuclear diatomics"
Chem. Phys. 95 (1985) 57.

55. D.J. Chornay, M.A. Coplan, J.A. Tossell, J.H. Moore, E.J. Baerends, A. Rozendaal

"Valence electron momentum distributions in $Cr(CO)_6$ from (e,2e) spectroscopy and SCF-MO calculations"
Inorg. Chem. 24 (1985) 877.

56. E.J. Baerends, P. Vernooijs, A. Rozendaal, P.M. Boerrigter, M. Krijn, D. Feil, D. Sundholm
"Basis set effects on the electron density and spectroscopic properties of CO"
J. Molec. Struct. (THEOCHEM) 133 (1985) 147.

57. A. Rozendaal, E.J. Baerends
"Analysis of σ-bonding, π-(back) bonding and the synergic effect in $Cr(CO)_6$. Comparison of Hartree-Fock and Xα results for metal-CO bonding"
in: Quantum Chemistry: The Challenge of Transition Metals and Coordination Chemistry, Ed. A. Veillard, D. Reidel Publ. Company, Dordrecht, 1986, pp. 159-177.

58. A. Rozendaal, E.J. Baerends
"The effect of internal vibration upon deformation densities and X-ray scattering intensities in H_2O and CO_2
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59. P.J. v.d. Hoek, A.D. Tenner, A.W. Kleyn, E.J. Baerends
"Hyperthermal alkali-ion scattering from a metal surface: a theoretical study of the potential"
Phys. Rev. B. 34 (1986) 5030-5042

60. P.H.M. Budzelaar, P.J.J.A. Timmermans, A. Mackor, E.J. Baerends
"Bonding in the ground- and excited states of Copper-alkene Complexes"
J. Organometallic Chemistry 331 (1987) 397-407

61. J.K. Olthoff, J.H. Moore, J.A. Tossel, J.C. Giordan, E.J. Baerends
"Anion states of η^4-olyene Iron Tricarbonyl Complexes"
J. Chem.Phys. 87 (1987) 7001-7006

62. P.M. Boerrigter, G. te Velde, E.J. Baerends
"Three-dimensional numerical integration for electronic structure calculations"
Int. J. Quantum Chem. 33 (1988) 87-113

63. L.J. Holleboom, J.G. Snijders, E.J. Baerends
"Natural Energy Orbitals and the One-particle Green's function"
Int. J. Quantum Chem. 34 (1988) 289

64. P.J. van den Hoek, W. Ravenek, E.J. Baerends
"The MSi_2/Si(111) (M=Co,Ni) Interface Chemical Bond"
Phys. Rev. Lett. 60 (1988) 1743

65. P.M. Boerrigter, E.J. Baerends, J.G. Snijders
"A relativistic LCAO Hartree-Fock-Slater investigation of the electronic structure of the actinocenes $M(COT)_2$, M = Th, Pa, U, Np and Pu"
Chem. Phys. 122 (1988) 357-374

66. G. Wiesenekker, G. te Velde, E.J. Baerends

"Analytic Quadratic Integration over the two-dimensional Brillouin Zone"
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Lausanne, Switserland, November 19, 2002

E.J. Baerends
The Kohn-Sham potential and Koopmans' theorem in DFT: on the pysical meaning of the components of the potential and on the relation between orbitals energies and ionization energies (Koopmans theorem in DFT) and exitation energies.
Conferende Universitaire de Suisse Occidentale. Commission scientifique pour l'enseignement du 3e cycle en chimie.
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E.J. Baerends
An MO interpretation of the excitation spectra of porphyrines and phtalocyanines on the basis of time-dependent DFT calculations.
Conferende Universitaire de Suisse Occidentale. Commission scientifique pour l'enseignement du 3e cycle en chimie.
Fribourg, Switserland, November 21, 2002

E.J. Baerends
Time-dependent DFT for response properties (polarizabilities, hyperpolarizabilities, excitation energies).
Conferende Universitaire de Suisse Occidentale. Commission scientifique pour l'enseignement du 3e cycle en chimie.
Geneve, Switserland, November 22, 2002

2003

E.J. Baerends
Time-Dependent Density Funcitonal Calculations for Excitation Spectra and other Respinse Properties
Journée calcul numerique intensif en Chimie et Physique,
Lille, France, March 6, 2003

E. J. Baerends
Time-dependent density functional calculations on the optical spectra of metal porphyrins and metal phthalocyanins
225th American Chemical Society National Meeting, Division of Computers in Chemistry, Symposium "Recent developments and applications of time-dependent DFT and related ab initio and semi-empirical methods"
New Orleans, USA, March 23-27, 2003

E. J. Baerends
The analog of Koopmans' theorem in DFT
225th American Chemical Society National Meeting, Division of Physical Chemistry, Symposium "New electronic structure methods: from molecules to materials"
New Orleans, USA, March 23-27, 2003

E. J. Baerends
A simple Ansatz for the full exchange-correlation hole and its application in a DFT functional dependent on occupied *and* virtual orbitals
Symposium "Electron correlation: ab initio methods and density functional theory"
Bad Herrenalb, Germany, July 16-19, 2003

E. J. Baerends
Car-Parrinello MD simulations of solvent effects on the oxidation catalysis by Fe(II) in water
MSC Seminar, Groningen, December 23, 2003

2004

E.J. Baerends
Time-dependent DFT applications to porphyrins and phthalocyanines: high accuracy combined with the simplicity of molecular orbital and fragment orbital analysis of the character and intensity ditribution of exitations.
Third International Conference on Porphyrins and Phthalocyanines
Los Angeles, USA, July 15, 2004

E.J. Baerends
Orbital-dependent functionals: Hartree-Fock, Kohn-Sham exact-exchange and beyond.
15th Canadian Symposium on Theoretical Chemistry.
Sainte-Adèle, Québec, Canada, July 12, 2004

E. J. Baerends
Avoided crossings, vibronic coupling and the issue of double excitations in TDDFT
International Conference: "Molecular Quantum Mechanics: The No Nonsense Path to Progress"
Cambridge, St. John's College, July 24-29, 2004

2005

E. J. Baerends
The analog of Koopman's theorem in DFT

International Nanoscience Workshop “Computatioinal Tools for Molecules, Clusters and Nanostructures”
Karlsruhe, Germany, January 23-26, 2005

E. J. Baerends
An energy decomposition approach to chemical bonding
Mariapfarr Winterschool,
Mariapfarr, 14-19 February, Austria, 2005

E. J. Baerends
Orbital-dependent functionals: exact exchange and beyond
Fritz Haber Institut der Max Planck Gesellschaft,
Berlin, April 20-22, 2005

E. J. Baerends
Dynamics of H_2 on stepped platinum surfaces"
Université de Marne la Vallée
Paris, June 16, 2005

E. J. Baerends
Orbital-dependent functionals: Hartree-Fock, Kohn-Sham exact-exchange and beyond
Université Pierre et Marie Curie,
Paris, June 23, 2005

E. J. Baerends,
42nd Meeting of the International Academy of Quantum Molecular Science
Recent developments in relativistic quantum chemistry
Menton, July 2-3, 2005

E. J Baerends
Why rough surfaces make good catalysts:
Reaction mechanisms of hydrogen on the Pt(211) stepped surface
Psi-k 2005 Conference
Schwäbisch Gmünd, September 17-21, 2005

2006

E. J. Baerends
Analysis of bonding and reactivity: from molecular systems to metal surfaces
Conference on “Recent developments in computational electronic structure theory”
Robinson college, Cambridge, UK
January 11-14, 2006

E. J. Baerends
Orbital dependent functionals: Hartree-Fock, Kohn-Sham exact-exchange and beyond
Princeton, USA
January 23, 2006

E. J. Baerends

Why rough surfaces make good catalysts:
Reaction mechanisms of hydrogen on the Pt(211) stepped surface
Rutgers University, New Jersey, USA
January 24, 2006

E. J. Baerends
De fysica van de chemische binding
Meeting Section of Physical Sciences, Royal Dutch Academy of Science
27 februari, 2006

E. J. Baerends
From DFT to DMFT and back
ICQC-12: 12th International Congress on Quantum Chemistry,
May 22-26, Kyoto, Japan

E. J. Baerends
Effects of porphyrin core saddling, meso-phenyl twisting and counterions on the optical properties of mesotetraphenylporphyrin diacids
ICPP-4: 4th International Congresss on Porphyrins and Phthalocyanines
July 3-7, 2006, Rome, Italy

E. J. Baerends
The role of the Fermi surface in molecule-metal bonding
1st European Chemistry Congress
August 26-31, 2006, Budapest, Hungary

E. J. Baerends
Avoided crossings on excited state surfaces and vibronic coupling in time-dependent DFT
Workshop on time-dependent density functional theory,
September 3-8, 2006, Benasque, Spain

E. J. Baerends
Analysis of bonding and reactivity: from molecular systems to metal surfaces
4th EFCATS School on Catalysis: Catalyst design: from molecular to industrial level
September 19-24, 2006, Sint Petersburg, Russia

E. J. Baerends
The first step in heterogeneous catalysis: simulation of molecular bond breaking at a metallic surface
SARA Superdag, 14 dec. 2006, Amsterdam, The Netherlands

2007

E. J. Baerends
Why rough surfaces make good catalysts: Reaction mechanisms of hydrogen on the Pt(211) stepped surface
Kolloquium für Physikalische Chemie, ETH Zürich
January 23, 2006, Zürich, Swizerland

E.J. Baerends
The role of the Fermi surface in adsorbate-metal interactions: an energy decomposition analysis
Bunsenkolloquium “Chemical Bonding in Position, Momentum, and Phase Space”
February 4-6, 2007, Konstanz, Germany

E. J. Baerends
Inspiration from Density Matrix Functional Theory: orbital dependent functionals for exchange PLUS correlation.
Seminar at Department of Chemistry, Cambridge University, Cambridge, UK
Feb. 28, 2007

E. J. Baerends
Oxidation catalysis by Fe(II) in water: AIMD simulations of FeO^{2+} generation; electronic structure and solvent effects
1st Georgian Bay International Conference on Bioinorganic Chemistry, Parry Sound, Ontario, Canada, May 22-25, 2007

E. J. Baerends
Time-dependent density functional theory for response properties
IDECAT Summer School “Computational methods for catalysis and materials science”
Porquerolles, France,
Sept. 15-27, 2007

E. J. Baerends
Density Functional Theory: basics and excitation energies
University of Technology, Eindhoven, The Netherlands
Dec. 3, 2007

2008
E. J. Baerends
Inspiration from density-matrix functional theory: orbital dependent functionals for exchange PLUS correlation, with an application to Van der Waals interaction
Symposium Prof. Ad van der Avoird, Nijmegen, The Netherlands, April 25, 2008

E. J. Baerends
Beyond the Independent Particle model. From Hartree-Fock to Density Functional Theory to Density Matrix Functionals
Mathematical Physics Seminar, University of Munich,
June 9, 2008

E. J. Baerends
The role of the Fermi surface in adsorbate-metal interactions: an energy decomposition analysis
VIII Girona Seminar: Aromaticity, basics and applications
Girona, Spain, July 7-10, 2008

E. J. Baerends
Excitation energies with time-dependent density *matrix* theory
International Symposium on Theoretical Chemical Physics VI,
Vancouver, Canada, July 19-25, 2008

E. J. Baerends
Density matrix functional theory
New-Zealand WATOC Satellite Meeting "Beyond the nonrelativistic Schrödinger equation – from the Dirac equation to electroweak theory"
Auckland, New Zealand, September 10-13, 2008

E. J. Baerends
The ADF program suite
World Association of Theoretically Oriented Chemists (WATOC)
Sydney, Australia, September 14-20, 2008

E. J. Baerends
Time-dependent density matrix theory: a solution to the problem cases of TDDFT?
Theory and Applications of Computational Chemistry (TACC)
Sjanghai, China, September 21-26, 2008

E. J. Baerends
Autumn Meeting in Computational Chemistry
Why rough surfaces make good catalysts: reaction mechanisms of hydrogen on the Pt(211) stepped surface
Kongsvinger, Norway, November 6-8, 2008

E. J. Baerends
Oxidation catalysis with the ferryl ion
Minisymposium Oxidation Catalysis
Groningen, The Netherlands, November 13, 2008

E. J. Baerends
How to catyalyze the oxidation of aliphatic C-H bonds? Electronic structure explanation of the role of the ubiquitous FeO^{2+} in oxidation reactions
HRSMC symposium, Amsterdam, November 27, 2008

2009

E. J. Baerends
How to catalyze the oxidation of aliphatic C-H bonds?
Chemistry Department Colloquium, Pohang University of Science and Technology, Pohang-si, South- Korea, April 24, 2009

E. J. Baerends
Time-dependent density functional theory
Seminars Center for Superfunctional Materials, Pohang University of Science and Technology, Pohang-si, South-Korea, May, 2009

E. J. Baerends
Excitation energies with time-dependent density *matrix* functional theory
13-th International conference on the Applications of Density Functional Theory in Chemistry and Physics
Lyon, France, Aug. 31 – Sept. 4, 2009

E. J. Baerends
The independent particle model
Seminars Center for Superfunctional Materials,
Postech, Pohang, South-Korea, Sept./Oct. 2009

E. J. Baerends
Kohn-Sham orbitals, Dyson orbitals and Koopmans' theorem in DFT
SWOCS Symposium/Workshop of Computational Sciences,
POSCO International Center, Pohang, South-Korea, Nov. 21,22, 2009

2010

E. J. Baerends
NRSC-Catalysis Peer Review Meeting
Heterogeneous and homogeneous catalysis: reactivity at steps in a metallic surface and reactivity at metaloxo groups
Eindhoven, The Netherlands, March 3, 2010

E. J. Baerends
Excitation energies with time-dependent density *matrix* functional theory
Deutsche Physikalische Gesellschaft Spring Meeting of the Condensed Matter Division,
Regensburg, Germany, March 22-26, 2010

E. J. Baerends
Excitation energies with time-dependent density *matrix* functional theory
Symposium of SPP: Modern and Universal first Principles Methods for Many-Electron Systems in chemistry and Physics
Bad Herrenalb, Germany, March 29 - April 1, 2010

E. J. Baerends
Density Matrix functional theory for energies, geometries and excitations
VII Conference on Electronic Structure, Principles and Applications (ESPA 2010)
Oviedo, Spain, June 28-July 2, 2010

E. J. Baerends
Response properties with time-dependent density *matrix* functional theory
IXth Girona Seminar, Girona, Spain, July 5-8, 2010

E. J. Baerends
The electron correlation problem in Theoretical Chemistry: where physics, chemistry and mathematics meet
Inaugural symposium of the Institute for Edge of Theoretical Science (IES),
Pohang, South-Korea, September 10, 2010

E. J. Baerends
Response properties with time-dependent density *matrix* functional theory

REHE
Beijing, China, September 24-30, 2010

E. J. Baerends
How to catalyze the 0xidation of aliphatic C-H bonds? Electronic structure explanation of the role of the ubiquitous FeO^{2+} in oxidation reactions
Invited seminar at Korean Advanced Institute for Science and Technology, Daejon, South-Korea, November 17, 2010

E. J. Baerends
Density *matrix* functional theory: a cure for DFT problems?
Pacifichem, Hawaii, USA, December 14-22, 2010

2011

E. J. Baerends
A perspective on density matrix functional theory for ground state and excited state potential energy curves
XV International Workshop on computational Physics and Materials Science:
Total energy and force methods
Abdus Salam International Centre for Theoretical Physics, Trieste, Italy, January 13-15, 2011

E. J. Baerends
Quantum Chemistry, from a historical perspective to modern applications
Invited seminar, Huzhou University, Huzhou, China, April 20, 2011

E. J. Baerends
Oxidation catalysis in chemistry and biology: how to improve on nature's FeO^{2+} based biocatalysts?
2nd Symposium on Enzymes and Biocatalysis - SEB 2011
Dalian World Expo Center, People's Rep. of China, April 25-29, 2011

E. J. Baerends
How to improve on Nature's FeO^{2+} based biocatalysts. O_2 activation through EDTA complexation
3d Georgian Bay International Conference on Bioinorganic Chemistry, CanBIC - III
Parry Sound, Ontario, Canada, May 31 - June 3, 2011

E. J. Baerends
Beyond DFT
CECAM workshop "How to speed up progress and reduce empiricism in DFT"
University College Dublin, Dublin, Ireland, June 20-24 2011

E. J. Baerends
Beyond DFT
Schrödinger Medal Lecture at Ninth Triennial Congress of the World Association of Theoretical and Computational Chemists
Santiago de Compostella, Spain, July 17-22, 2011

E. J. Baerends
XVIIth Congress of the International Society for Theoretical Chemical Physics, ISTCP-VII
Excitations in DFT and DMFT. Time-dependent DFT and DMFT.
Waseda University, Tokyo, Japan, September 2-8, 2011

E. J. Baerends
Why rough surfaces make good catalysts. Reaction mechanisms for H_2 dissociation on the Pt(211) stepped surface
SWOCS-III, Symposium/Workshop of Computational Sciences,
POSCO International Center, Pohang, South-Korea, Nov. 19, 2011

E. J. Baerends
Reactivity at surfaces. Scattering, trapping and reaction.
Meeting of the Finnish Centre of Excellence in Computational Molecular Science,
Helsinki, Finland, Dec. 2, 2011

2012

E. J. Baerends
Why rough surfaces make good catalysts: reaction mechanisms of hydrogen molecules on the Pt(211) stepped surface
Colloquium for the NTH School for Contacts in Nanosystems,
TU Clausthal, Clausthal, Germany, January 19, 2012

E. J. Baerends
Molecular properties from density matrix response
Conference on “Challenges in Density Matrix and Density Functional Theory”
Ghent, Belgium, April 1-6, 2012.

E. J. Baerends
A perspective on density *matrix* functional theory for ground state and excited state energy surfacs
QSCP-VII, 17th Workshop on Quantum Systyems in Chemistry and Physics,
at Åbo Akademi, Turku, Finland, August 19-25, 2012

E. J. Baerends
Density matrix functional theory of Van der Waals interactions
International Conference “Quantum Chemistry in the Solid State. Magnetic Coupling and Excited States.”

Groningen, The Netherlands, Aug. 31 -September 1, 2012

E. J. Baerends
Density matrix functional theory of Van der Waals interactions
TACC-2012: Conference on Theory and Applications of Computational Chemistry
Pavia, Italy, September 2-7, 2012

E. J. Baerends
Excitation energies from density matrix response
Symposium/Workshop of Computational Sciences IV
Pohang, South Korea, Nov. 17, 2012

2013

E. J. Baerends
Molecular properties from density MATRIX response
Sanibel Symposium on Quantum Theory of Electronic Structure, Spectra and Dynamics, St. Simons Island, Georgia, USA, Feb. 17-22 2013

E. J. Baerends
Beyond DFT: density *matrix* functional theory for ground and excited state energy surfaces
Korean Physical Society Meeting, Korea Advanced Institute for Science and Technology, KAIST, Daejeon, South-Korea, April 25, 2013

E. J. Baerends
Density Functional Theory and Beyond
Lecture Course on the occasion of KAIST Chemistry International Summer Lectureship Award, Korean Advanced Study Institute (KAIST), Daejeon, South-Korea, May 26 - June 1, 2013

E. J. Baerends
Why rough surfaces make good catalysts: reaction mechanisms of hydrogen molecules on the Pt(211) stepped surface
KAIST Chemistry Lectureship Award, Korean Advanced Study Institute (KAIST), Daejeon, South-Korea, May 31, 2013

E. J. Baerends
Towards a natural orbital functional for Van der Waals bonding
CECAM workshop on "Density functional theory:
learning from the past, looking to the future",
Berlin, Germany, July 2-5, 2013

RESEARCH OVERVIEW

E. J. Baerends

A) Summary of research interests.

1) Many-electron theory, in particular the density functional theory (DFT) for many-electron systems.

2) Development of time-dependent DFT and application to response properties such as (hyper)polarizabilities, Raman intensities, Electronic and Vibrational Circular Dichroïsm etc., and notably excitation energies.
3) Density matrix functional theory and time-dependent density matrix functional theory.
4) Understanding, explaining and predicting properties of molecules and (transition-metal) complexes from their electronic structure. Studies of structure, bonding and reactivity (homogeneous catalysis).
5) Relativistic effects in the chemistry and spectrosopy of heavy element compounds.
6) Surface-molecule interactions: scattering from and dissociation at metallic surfaces of small molecules (heterogeneous catalysis).
7) Solvent effects on reactivity by *ab initio* (DFT) molecular dynamics (Car-Parrinello) simulations.
8) Development and implementation of new computational techniques, mostly based on density functional theory: the Amsterdam Density Functional programme system
9) Development of analysis methods and concepts for bond energies and for molecular charge distributions. Elucidation of the role of Pauli repulsion and of the kinetic energy in the formation of chemical bonds, the height of transition barriers, and the formation of metal-molecule bonds and molecular dissociation over metallic surfaces.

B) Summary of Research Achievements.

1. Thesis: "Self-consistent molecular Hartree-Fock-Slater Calculations" and related papers, Refs. [1-11].
This work consists of the development of the now universally employed methodology for DFT calculations, using a combination of three ingredients: a) the conventional expansion method of quantum chemistry ("basis sets") for the Kohn-Sham orbitals; b) the use of auxiliary functions (called "density fitting," or "resolution of the identity") for the Coulomb potential evaluation; c) 3D numerical integration for calculation of (parts of) the Hamiltonian matrix elements. It built on the pioneering work of D. E. Ellis with the so-called Discrete Variational Method (DVM). It is at the basis of the present Amsterdam Density Functional program suite.
ad b). At the time of its development (1973) only a very approximate method (the so-called scattered wave Xα method), was available for calculations on molecular systems with the Slater exchange-correlation functional (at that time called Hartree-Fock-slater or Xα). This method involved spherical averaging of the electronic potential in each atomic domain, thus precluding the calculation of reliable total energies. Bond energies and bond lengths could not be obtained, and in particular the spherical averaging wiped out all directional properties ("linear water").

The density fitting was introduced for the first time as a technique to scale down the two-electron integral evaluation "bottleneck" from its n^4 scaling (n is the number of basis functions) to n^3. In fact, since the fitting was done per atom pair, this step was n^2 scaling, although the total Coulomb problem remained n^3 scaling. It has often been commented that DFT (Kohn-Sham) is "of course" n^3 scaling, but this is not

correct: the traditional evalaution of the Coulomb operator matrix elements of the Kohn-Sham hamiltonian, would make the Kohn-Sham DFT calculations n^4 scaling. With the added complication of a numerical evaluation of the exchange-correlation matrix elements, Kohn-Sham calculations would have been more expensive than Hartree-Fock calculations, the density fitting was essential to give DFT the appeal of a much faster method for large systems.

The density fitting has been adopted in a regular Gaussian orbital based quantum chemistry code for DFT calculations by Sambe and Felton in 1975. The Sambe and Felton code has been the basis for further development by Dunlap, Connolly and Trickey, who introduced an improved fitting for total energy calculations ("variational fitting") in 1979. Density fitting has been an essential element of the major DFT codes, both our code based on STO basis functions (ADF) and the ones based on Gaussian basis functions such as DMon, DGauss and later Turbomole. After the upsurge of interest in DFT in the quantum chemistry community in the nineties, this particular computational approach to more favorable scaling of the calculations has also been adopted for Hartree-Fock calculations and correlated calculations (MP2).
ad c) The numerical integration was originally taken over from the work of D. E. Ellis (Diophantine integration). In the mid eighties a new numerical integration method has been developed which was based on a partitioning of space into domains (spheres and (truncated) pyramids) over which integration with product Gauss rules could be carried out to arbitrary precision (Refs. 62, 109). This so called *Voronoi cell method* is arguably the most accurate 3D numerical integration method today and is still used in the ADF program. Becke's integration method, which appeared simultaneously, is easier to implement and is more widely used.

The HFS/ADF method uses numerical integration over all matrix elements of the one-electron Hamiltonian (the Kohn-Sham Hamiltonian). This allows the use of Slater-type-orbital (STO) basis sets, which are more efficient (fewer are needed for basis set convergence).
This work has been instrumental to keep alive the interest in DFT in the quantum chemistry community, when in the mid seventies it became clear that the multiple scattering Xα method was failing for molecules, notably for geometries (linear water!) and for bond energies. The muffin tinning of the electronic potential is a too severe an approximation for molecules. Our "full potential", basis set based method showed that the performance of Xα was very good for molecular geometry and energy. Moreover, the excitation energy calculations, performed at the same with the ΔSCF method, showed surprisingly good agreement with experiment for transition metal complexes.

The ADF (for *A*msterdam *D*ensity *F*unctional) program system has been developed over the years into a very comprehensive program system (see Refs. 210, 262). It is capable of handling large systems such as transition-metal complexes and clusters, large organic systems (several base pairs of DNA), large inorganic systems (cubic molecular nano-containers as selective fullerene hosts), periodic systems (3-, 2- or 1-dimensional) and heavy element compounds (relativistic effects). Many properties have been implemented

over the years, both by the Calgary group (T. Ziegler) and the Amsterdam group (E. J. Baerends): frequencies, geometry optimization and transition state search, NMR, ESR, Polarizabilities, Hyperpolarizabilities, Excitation energies, Raman intensities, Electronic Circular Dichroïsm, Vibrational Circular Dichroïsm.

2) The first method to do excitation energy calculations in DFT emerged from the work done together with Tom Ziegler (at that time graduate student at Calgary) in 1976 (Refs. 12,13). This was a straightforward ΔSCF method where excited states were represented with excited determinants. This was worked out into a scheme for multiplet splitting calculations. It has remained the only method for this type of calculation till the advent of time-dependent DFT in the mid nineties.

3) Relativistic effects have in our work been first addressed by perturbation theory (in a "coupled" form) (with J. G. Snijders in the late seventies (20,24,27,29,31,32,40) and with P. M. Boerrigter and others (45, 65) in the eighties). Amongst the studies of relativistic effects, an early important result has been the "Dutch revolution" of reinterpretation of the origin of the relativistic contraction of bond lengths (27,29,31). They are not due to contraction of the radius of valence AOs but are due to a softening of the inner repulsive wall in the *E vs R* curves due to the effect of the mass-velocity relativistic correction to the kinetic energy.
In general this work has much contributed to elucidation of the origin of relativistic effects. In the early work the perturbation formalism allowed for detailed analysis. It was shown that it is not true that relativistic effects only work on the (high-speed) core electrons, and then influence the valence electrons by e.g. the contraction of the core orbitals. "Direct" relativistic effects proved to be important for valence electrons also. A detailed account of the origin of relativistic effects has been given in a later publication with Schwarz (81).

4) The importance of so-called picture change effects for the correct calculation of properties within a two-component formalism has been identified (see E. J. Baerends, W. H. E. Schwarz, P. Schwerdtfeger and J. G. Snijders, J. Phys. B: At. Mol. Opt. Phys. 23 (1990) 3225). This is a subtle and important issue, since it greatly influences the value that is obtained for properties that are heavily weighted towards the nucleus (e.g. $1/r^3$ dependence), such as electric field gradients. This has played a large role in recent years in electric field gradient calculations, e.g. by Sadlej and coworkers and by ourselves (241). Often, electric field gradient calculations at the nucleus are the only means (or the most reliable means) to get to know the nuclear quadrupole moment.

5) Later (in the nineties) a two-component regular hamiltonian method has been developed. The full four-componetn Dirac equation is too computationally demanding. The use of the Pauli hamiltonian in a non-perturbative manner, is fairly successful in frozen-core calculations, but eventually breaks down when very flexible basis sets are used. The in-house developed and now much applied zero-order regular approximation (ZORA) (with E. van Lenthe) affords a very efficient solution to the two-component equations to which the Dirac equation can be transformed (111, 119, 120, 127, 136, 145, 147, 168, 172, 223, 301). This has put two-

component relativistic variational calculations on a firm basis. The calculations are - owing to the numerical integration technology of ADF - very efficient, making relativistic calculations (without spin-orbit coupling) as cheap as nonrelativistic ones.

6) Fundamental studies of the connection between the DFT approach to electron correlation and the traditional insights based on density matrices have enabled the expression of the key quantities of DFT (exchange-correlation energy density and Kohn-Sham one-electron potential) in terms of wavefunction derived quantites, notably the conditional amplitude. This has made it possible to relate conspicuous features in the KS potential, such as the hump at intershell boundaries in atoms, and the peak at the bond midpoint in stretched molecules, to electron correlation phenomena. In particular the behavior of the Fermi hole and the Coulomb hole as a function of the position of the reference electron around which the hole is considered, is responsible for these features in the KS potential. On the fundamental theoretical side, this connects Kohn-Sham DFT directly with exact wavefunctions and correlation calculations. See Refs. 76, 118, 124, 126, 131, 140, 141, 143, 144, 149,, 153, 155, 162, 163, 167, 173, 174, 181, 185, 196, 199, 202, 205, 208, 229, 242, 249, 250, 269, 271, 282, 343, 364) and the review (192).

7) An important result has been the recognition of the importance of the Coulombic decay of the Kohn-Sham potential (118). This has led to the first demonstration that the proper asymptotic decay of the Kohn-Sham potential is crucial for obtaining accurate response properties such as (hyper)polarizabilities (165). It has subsequently led to the development of new functionals for the Kohn-Sham potential, integrating the findings mentioned under point 5) with the proper asuymptotic decay of ref. (118), which greatly improve the calculation of response properties, including Rydberg excitations. Model potentials have been proposed like SAOP (222, 236, 237) and GRAC (258) that perform excellently in many response property calculations (258, 270).

8) The established connection between DFT and wavefunction theory has also afforded the derivation in DFT of the analogue of Koopmans' theorem for the Kohn-Sham one-electron energies (275, 293, 295 306, 316). This theorem, establishing the connection between one-electron energies and ionization energies, is well known in Hartree-Fock theory. This connection has long been denied in DFT, but it proves to hold much more accurately in DFT than in Hartree-Fock theory. This is very important for the use of Kohn-Sham MO theory as a qualitative MO method in chemistry.

9) A major interest has been the development and use of bond energy analysis tools and concepts. This has been applied mostly in the context of the Morokuma energy decomposition method, with the important change that usually the polarization and charge transfer terms have been replaced by the symmetry based partitioning (e.g. σ and π bonds) afforded by Ziegler's extended transition state method. This energy decomposition has been used to build up more detailed understanding of chemical bonding, notably the effect of electrostatic (potential energy) effects and the kinetic energy effects (see review Ref. 245). This

is done in the context of Kohn-Sham MO theory, which establishes the Kohn-Sham MO theory as a fully fledged chemical theory for structure and bonding. The theoretical basis for this use of Kohn-Sham theory can be found in the theoretical work described under point 3). Many applications to chemically interesting systems and problems have been published (303).

10) The development and implementation in the eighties of a highly accurate method for electronic structure calculations on periodic systems, has proven to be extremely useful for the generation of very reliable potential energy surfaces for surface-molecule interaction. A breakthrough in the theoretical modeling of surface-molecule interactions, which is very important for reactivity at surfaces (heterogeneous catalysis, corrosion) has occurred by the performance of dynamics calculations (by the collaboration with G. J. Kroes) on these very accurate potential energy surfaces, yielding a complete description of all scattering and dissociation channels. see Refs. (135, 150, 156, 159, 171, 186,190, 191, 195, 206, 211, 215, 219, 221, 232, 251, 252, 256, 268, 273, 278, 279, 288, 292, 298, 327, 328, 334, 340, 351, 357,362, 380)

11) Implementation of time-dependent DFT based response methods, in combination with functional development based on theoretical work (see 5) have enabled the calculation of many spectroscopic properties of (large) molecules, with very gratifying accuracy, see Refs (139, 164, 165, 183, 184, 204, 212, 213, 214, 225, 226, 227, 228, 231, 236, 237, 238, 243, 250, 254, 258, 270).
We have discovered and extensively studied the very important failure of time-dependent DFT (in its present adiabatic implementation) in the case of long chain-like molecules. There is even a divergence with chain length of LDA and GGA methods of DFT for polarizability and notably hyperpolarizability calculations of chain-like molecules (polymers!) (184, 212, 226, 243)

12) Solvent effects on reactivity at a transition-metal center are being studied with Car-Parrinello molecular dynamics, which reveal in a striking manner the importance of the H-bond networks in water for reaction mechanisms. A major research effort has been directed in recent years to homogeneous catalysis problems, notably the industrially and environmentally very important oxidation catalysis. We have theoretically established that in the Fenton chemistry (oxidation with hydrogen peroxide catalyzed by Fe^{2+} ions in water solution) the reactive intermediate is most probably not the widely postulated $OH^{\bullet}$ radical but the FeO^{2+} moiety (264, 265, 308, 314, 322, 370, 371. 376, 378) This connects Fenton chemistry with the biologically important P450 enzymes.

13) Recently we have concentrated on the development of density matrix functional theory (DMFT), and aalso the time-dependent variant, TDDMFT. Important progress has already been made, both in the development of functionals for ground state properties (277, 286, 299, 348, 350, 352, 365, 366, 367), and for excited states (373, 381, 382). It is very promising that the three notorious problem cases of TDDFT - excitations at stretched bond length, charge transfer excitations and double excitations - are all solved in model calculations with time-dependent DDMFT for two-electron molecules.