António Joaquim de Campos Varandas

CURRICULUM VITÆ

COIMBRA
May 2013

Personal

Born: September 19, 1947
Place of birth: Mata-Curia, Portugal
Nationality: Portuguese

Address

Departamento de Química
Universidade de Coimbra
3049 Coimbra Codex, Portugal
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Education and degrees

1965-67: Universidade de Coimbra, Portugal.
Bachelor in Chemical Engineering.
1967-70: Universidade do Porto, Portugal.
1970-71: Industrial training at Companhia Portuguesa de Celulose,
Cacia. Diploma in Chemical Engineering, with distinction.
1973-76: University of Sussex, England. Ph.D. in Theoretical Chemistry.
Thesis: "Studies on Potential Energy Surfaces".
Supervisor: Professor John N. Murrell.
November
1976: Equivalence of Ph.D. to the degree of Doctor in Sciences
(Chemistry) by Portuguese Universities.
May 1984: Professor Agregado (by unanimity).
May 1988: Full Professor (ranked first).

Academic fellowships

1965-70: Fundação Calouste Gulbenkian scholarship
1973-76: NATO scholarship
July-
September 1978: British Council bursar

Visiting professor

August 1983: Max-Planck-Institut für Strömungsforschung,
Göttingen, Germany.

August 1985: University of Minnesota, United States of America.
October 1985: *Professeur Associé* at the Laboratoire de Mécanique Ondulatoire Appliquée, Université de Reims, France.
May-October 1988: Invited Professor and Visiting Research Scholar of the Minneapolis Supercomputer Institute at the University of Minnesota, United States of America.
June-July 1995: Invited Professor and Cherry L. Emerson Fellow at the Department of Chemistry of Emory University, Atlanta GA, United States of America.
May-June 2005: Invited Professor at Dalian Institute of Chemical Physics of Chinese Academy of Sciences (Dalian, P.R. of China).

Full-time professional experience

1965-67: Monitor ("tirocinante") at Centro de Estudos de Química Nuclear e Radioquímica, Universidade de Coimbra.
1971-73: Assistant Professor, Universidade de Coimbra.
1977: Auxiliary Professor, Universidade de Coimbra.
June 78-March 79: Army service in the Navy.
1982: Associate Professor, Universidade de Coimbra.
Maio 1988: Full Professor, Universidade de Coimbra.

Academician

2006-: Corresponding member of the Academia de Ciências de Lisboa (Portugal).

Honorific positions

September 1998-: Honorary Professor (*Profesor Invitado*), Instituto Superior de Tecnologias y Ciencias Aplicadas† (La Habana, Cuba)
June 2005-, Guest Professor of the Dalian Institute of Chemical Physics, Chinese Academy of Sciences, (Dalian, P.R. China)
July 2006-: Honorary Professor of Physics at Henan Normal University, (Henan, P.R. of China).

† Formerly, Instituto de Ciencias y Tecnologia Nucleares.

Teaching

Undergraduate courses taught:
General chemistry

Physical chemistry I†
Chemical kinetics
Solid state chemistry†
Molecular physical chemistry†
Quantum chemistry
Computational chemistry
Theoretical & structural chemistry
Theoretical chemistry
Statistical mechanics
† In collaboration.

Supervision of many Diploma thesis in Chemistry.

Graduate teaching in MSc courses at:
Universidade do Porto (1980)
Universidade de Lisboa (1988)
Universidade de Coimbra (1982-2005)
Universidade Agostinho Neto, Luanda, Angola (May-June 2013)

Coordinator of mini-course entitled "From molecular structure to potential modeling" for postgraduates in Physics at Departament of Physics Universidade Federal do Espírito Santo (Brazil, 2012)

Member of accompanying committee of Master Diogo Fialho de Almeida, Ph.D. student in Molecular Physics at Universidade Nova de Lisboa under the supervision of Doctor Paulo Limão Vieira.

Appointed as examiner of numerous MSc and Ph.D. theses in Chemistry and Physics, both in Portugal and abroad (Spain, France, Cuba, India).

Belonged to numerous national university panels for academic promotion both in Chemistry and Physics.

National coordinator of Erasmus ICP CH-3012/13 network involving the University of Coimbra and six other european universities (1995/96).

Graduate thesis supervision and research associates[‡]

Ph.D. and M.Sc.:

Manuel A. Matías (Salamanca, Spain), Ph.D., 1990.
Victor M.F. Morais (Porto, Portugal), M.Sc., 1984; Ph.D., 1990.
Luís A.M. Quintales (Salamanca, Spain), Ph.D., 1991.
João C.P.P. Brandão (Coimbra, Portugal), Ph.D., 1993.
Alberto A.C.C. Pais (Coimbra, Portugal), M.Sc., 1987; Ph.D., 1993.
Ana Maria A. Rodrigues (Coimbra, Portugal), M.Sc., 1993.
Jorge M.C. Marques (Coimbra, Portugal), Ph.D., 1995.
Wenli Wang (Coimbra, China), Ph.D., 2000.
Sérgio P.J. Rodrigues (Coimbra, Portugal), Ph.D., 2000.
Zong-Rong Xu (Chengdu, China), Ph.D., 2001.
Antonio Riganelli (Perugia, Italy), Ph.D., 2001.
Lei Zhang (Chengdu, China), Ph.D., 2003.
Jorge L. Llanio-Trujillo (Pinar del Río, Cuba), Ph.D., 2003.
Pedro J.B.S. Caridade (Coimbra, Portugal), M.Sc. 2003, Ph.D., 2004.
Paulo E. Abreu (Coimbra, Portugal), Ph.D., 2005.
Vera Mónica de Oliveira Batista (Coimbra, Portugal), MSc., 2006.
Osvaldo B.M. Teixeira (Cidade da Praia, Cabo Verde), MSc., 2006.
Luis Poveda (Santiago de Cuba, Cuba), Ph.D., 2007.
Mihail Cernei (University State, Moldova), Ph.D., 2008.
Luis P. Viegas (Coimbra, Portugal), Ph.D., 2008.
Maikel Ballester Furones (Dep. Physics, Univ. La Habana, Cuba), Ph.D., 2008.
Vinicius C. Mota (Univ. de Minas Gerais, Brazil), Ph.D., 2008.
Saju Joseph, (Mahatma Gandi University, Kottayama, India), Ph.D., 2011.
Yuzhi Song (Dep. of Physics, Shandong Normal University, China), Ph.D., 2011.
Yongqing Li (Dep. of Physics, Lianoning University, China), Ph. D., 2012.

Current postgraduate students, and expected completion dates:
Osvaldo B.M. Teixeira$\star\star\star\star\star$ (Cidade da Praia, Cabo Verde), Ph.D., 2010.
Breno Rodrigues Lamaghere Galvão (Univ. de Minas Gerais, Brazil), Ph.D., 2012.
Jing Li (College of Physics and Electronics, Shandong Normal University, Shandong, Jinan, PR China), Ph.D., 2013.

Postdoctoral associates:

Mercedes R. Pastrana (Valladolid, Spain), October 1988-December 1989.
Gennady V. Mil'nikov (Moscow, Russia), July 1995-March 1996; July 1996; June 1997-December 1998.
Pedro Jimeno (Madrid, Spain), March 1997-March 1998.

Raul González-Jonte Cruz (Pinar del Río, Cuba), October 1997-October 1998 October 1998.
Itamar Borges Jr. (Rio de Janeiro, Brazil), September 1999-September 2000.
Frederico V. Prudente (Brasília, Brazil), September 1999-September 2001.
Eric Kolesnick (Academy of Sciences, Moldova), April 2000-December 2000.
Emilio Martínez-Núñez (Santiago de Compostela, Spain), September 1999-December 2000.
António F. Ramos (Santiago de Compostela, Spain), January-December 2001-.
Alexander Alijah (Bielefeld, Germany), September 2001-.
Lei Zhang (Chengdu, China), May 2003-May 2005.
Jorge L. Llanio-Trujillo (Pinar del Río, Cuba), May 200-.
Eugene S. Kryachko (Academy of Sciences of Ukraine, Kiev, Ukraine), January-March 2003.
Malgorzata Biczysko (Wroclaw, Poland), February 2004-2006.
Pedro J.B.S. Caridade (Coimbra, Portugal), August 2004-.
Flávia Rolim de Almeida (Belo Horizonte, Brazil), November 2004-2005, January 2007-December 2007.
Juan Carlos Juanes-Marcos (Nottingham, U.K.). April 2005-2006.
Geórgia Maria Amaral Junqueira** (Univ. Fed. Juiz de Fora, Brazil), March 2007-2008.
Biplab Sarkar (Department of Chemistry, North-Eastern Hill University Shillong, India), February 2009-August 2010.
Luis P. Viegas (Coimbra, Portugal), Ph.D., 2008.
Vinicius C. Mota (Univ. de Minas Gerais, Brazil), Ph.D.†, 2008.
Tanmoy Mondal (School of Chemistry, University of Hyderabad Hyderabad, India), February 2011-.
Muhammad R.S.A Janjua (University of Sargodha, Sargodha, Pakistan), April 2011-May 2012.
Yuzhi Song (Dep. de Quimica, Universidade de Coimbra, Portugal), January 2011-December 2012.
Ulises Miranda‡, (Univ. Autonoma de Mexico, Mexico), May 2012-.
Rahul Sharma, (Indian Association for the Cultivation of Science, Kolkata, India), January 2013-.

†With a grant from Consejo Nacional de Ciencia y Tecnología (CONACYT) of Mexico.
‡Reconhecido como grau de Doutor em Física pela Câmara de Pós-Graduação da Universidade de Minas Gerais (Julho 2012).

Visiting professors/researchers/other:†
Roman Nalewajski (Jagiellonian University, Cracow, Poland),

October-November 1992)

Henrik Szichman (Soreq, Yavne, Israel), October-November 1993; October-December 1996; September-December 1999.

Anatoli I. Voronin (Russian Academy of Sciences, Moscow), February 1994-April 1995; March-July 2000.

Huagen Yu (Academia Sinica, Chengdu, China), March 1995-March 1996; May 2000.

Juan D. Garrido (ISCTN, La Habana, Cuba), October 1998-March 1999; October 1999-February 2000, October 2000-February 2001.

Michael Baer (Sorec, Yavne, Israel), January-April 1999.

Alexander Alijah* (Bielefeld, Germany), March-October 1999.

Jesus A. Sabin del Valle (ISCTN, La Habana, Cuba), March-September 2000.

Heshel Teitelbaum (University of Ottawa, Canada), July-August 2002.

Wazir-ul H. Ansari (LN Mithila University, Darbhanga, India), December 2001-June 2002.

Piotr Piecuch (Michigan State University, East Lansing, U.S.A.), March-May 2006.

Ke Li Han (Chinese Academy of Sciences, Dalian, China), September 2006.

Juana Zoila Junco Horta (Universidad Camilo Cienfuegos de Matanzas, Cuba), August 2006-February 2007.

Agustin Corzo-Espinoza (Universidad Camilo Cienfuegos de Matanzas, Cuba), September 2007-February 2008.

Raul Palmeiro Ulriach*** (Universidad de Alcalá de Henares, Spain), June 2008-August 2008, June 2009-August 2009, June 2009-August 2010,

Sujitha Kolakanty**** (IIT Kanpur, India), October-November 2008.

Saurabh Srivastava**** (IIT Kanpur, India), September-November 2009; November-December 2010.

Satrajit Adhikari (Physical Chemistry Department I.A.C.S, Jadavpur-700 032, Kolkata, India), August 20-October 20, 2010; June-August, 2011;

Marlies Hankel (Centre for Computational Molecular Science, The University of Queensland QLD 4072 Brisbane, Australia), August 22-September 18.

Agastya P. Bhati, Indian Institute of Science Education and Reserach, Mohali, Punjab, India (as Summer Internship, July-August 2012)).

‡ In parenthesis is the home address or University address previously to coming to Portugal.

⋆With a grant from INIDA (Germany).

⋆⋆With a grant from CNPq (Brazil).

⋆ ⋆ ⋆With a grant from Universidad de Alcalá de Henares (Spain).

⋆ ⋆ ⋆⋆With a grant from project GRICES.

⋆ ⋆ ⋆ ⋆ ⋆In co-supervision with J. Garcia de La Vega (UAM, Mardrid).

Research (update 2005)

My research interests have focused on theoretical studies of molecular systems, covering both energetic and dynamics aspects. In addition to fundamental research, I have been involved in the application of theoretical methods to specific systems of practical interest. Some examples of the progress that I and my collaborators have made on specific problems are highlighted in the following paragraphs.

Early studies focused on perturbation theory. We developed a variation-perturbation method for dynamic polarizabilities, and a new perturbative approach to the potential energy curves of rare gas dimers in the region of the van der Waals minimum. The method, which combines first-order exchange perturbation calculations with a realistic second-order dispersion interaction, has been a precursor of successful semiempirical approaches in use today.

The calculation and modeling of potential energy surfaces using the methods of quantum mechanics are topics of extreme importance in theoretical chemical physics. Since my Ph.D. studies, I have employed both *ab initio* and semiempirical methods to calculate such surfaces. Amongst the early *ab initio* studies, I emphasize the identification of a conical intersection in the potential surfaces of LiNaK using the theorems[1] due to Longuet-Higgins. The approach is frequently used today to identify such intersections.

In the field of potential energy surfaces for reaction dynamics, I developed with J.N. Murrell and other Colleagues a general strategy known as the many-body expansion (MBE), a method which has since afforded great popularity amongst dynamicists. In 1984, I proposed a double many-body expansion (DMBE) theory. While keeping much of the simplicity of MBE, the DMBE theory has a stronger physical basis, and covers in a formally correct way the complete configuration space of the molecule. The DMBE

[1]Of relevance here is the first theorem which states that a real adiabatic wave function changes sign when transported adiabatically along a closed loop that encircles the conical intersection.

theory has been shown to handle both chemically stable molecules and less stable complexes of the van der Waals type. Indeed, some of the most accurate potential energy surfaces currently in use for well known benchmark systems such as[2] H_3 and HO_2 are of the DMBE type. In 1995, the DMBE method was extended to multi-sheet potential energy surfaces for molecules with atoms of any spin multiplicity and angular momentum[3].

An important requirement of DMBE is to know the dependence of dispersion coefficients on the intramolecular coordinates of the participating subsystems, a requisite in turn essential if the potential is to be used to interpret experimental data where the vibrational coordinates of the interacting subsystems are involved. Focusing on this, we have proposed and tested new semiempirical techniques for the evaluation of such coefficients. We have also developed virial theorem constraints for the n-body energy terms of potential energy surfaces, and used the virial theorem to decompose such surfaces and assess their reliability.

In reaction dynamics and kinetics[4], we have used both classical and quantum mechanical methods. While such studies served as tests on the adequacy of our own surfaces, some focused in reactions with relevance in areas of practical interest such as atmospheric chemistry and combustion processes. We have also developed and tested classical capture theories, and accounted for recrossing in exothermic reactions proceeding over barrier-free potential energy surfaces with deep wells. Moreover, we suggested a new method for quasiclassical trajectories on local potential energy surfaces defined from gradients and Hessians, thus avoiding a global potential energy surface. We have also investigated the so-called zero-point energy problem of classical dynamics, and proposed and tested both 'active' and 'nonactive' schemes as fixes to the leakage of zero-point vibrational energy in trajectory calculations. In 1995, I have proposed a method to extract the cross section from quantum mechanical reactivities calculated for zero total angular momentum. This is important to extrapolate the results of accurate quantum calculations, which are seldom viable for situations involving non-zero total

[2]Published in 1987 and 1990, respectively.

[3]The formalism has been generalized in two review articles published in 2000 and 2004.

[4]The rationalization of kinetics data without focusing on the detailed dynamics has also an important role in chemistry. Within this context, we have proposed an intersecting state model which assumes that the bond-orders of the breaking and forming bonds do not always sum to unity. Recent *ab initio* studies supported the prediction that total bond-order may not be conserved during an elementary reaction.

angular momentum. Sarting in 1996, we developed a general theory to include tunnelling effects into quasiclassical trajectory calculations.

The major areas of my research in the past few years reflect a consistent continuation of previous work, focusing on four major topics: (a) *ab initio* calculation and modelling of potential energy surfaces; (b) generalization of the Born-Oppenheimer approximation to molecular systems with electronic degeneracies; (c) dynamics (classical and quantum) of reactions with relevance in atmospheric chemistry and combustion processes; (d) direct methods for the calculation of partition functions. The following surveys some of the major developments achieved thus far. In (a), besides *ab initio* calculations for specific systems, I developed[5] a semi-theoretical approach to extrapolate the correlation energy to the complete basis set limit. I have also proposed an 'energy-switching' method to construct global potential energy surfaces of spectroscopic accuracy at regions where such an accuracy is known from experimental work. Alternatively, we have shown how to refine a DMBE surface to attain spectroscopic accuracy via a multiproperty fit which includes such a data[6]. In (b), we reported detailed quantum studies of vibrational spectroscopy for the 'trough' and 'cone' states of H_3 (and its isotopomers) and Li_3 both with consideration and without consideration of the so-called geometric phase effect. Most recently, we have extended such calculations to study the ro-vibrational spectroscopy of the interstellar H_3^+ ion in its triplet state. A proper assignment of all calculated ro-vibrational levels for values of the total angular momentum up to $J = 10$ (*i.e.*, the lowest 19 bands) has been presented. Their estimated accuracy of 0.1–0.3 cm^{-1} may therefore stimulate experiments aiming at their observation in astrochemistry and hydrogen plasmas. Although the geometric phase effect turned out to have little effect for the trough states in the lowest triplet sheet, it plays a crucial role for those in the upper sheet. However, the novelty has perhaps been the development of new single-surface equations to carry out GP calculations by using the 'mixing angle'[7] to represent the geometric phase. Also noteworthy is our most recent work on cyclic phases at N-fold Jahn-Teller degeneracies, where it has been shown for the first time that the GP effect is a property inherent to inversion of the adiabatic electronic wave vectors

[5] A semiempirical method (with acronym DMBE-SEC) to scale the external correlation energy such as to reproduce the limit of complete one-electron basis set and full configuration-interaction expansion has also been suggested in 1989.

[6] Note that the DMBE or ES surfaces obtained by using experimental data for their calibration contain information beyond the usual Born-Oppenheimer approximation.

[7] This is the angle which diagonalizes the potential matrix.

in the N-dimensional wave-vector space. The salient features in (c) are perhaps the detailed study of the reactions $H+O_3 \rightarrow OH+O_2$ (and its reverse), $OH + O_3 \rightarrow O_2 + HO_2$ (and its reverse), $HO_2 + O_3 \rightarrow OH + 2O_2$, and the suggestion that the reverse $OH(v')+O_2(v'')$ and [8] $O_2(v')+HO_2(\mathbf{v})$ reactions may offer clues for ozone related problems [9] in the middle atmosphere under plausible conditions of local thermodynamic disequilibrium (commonly referred to as non-local thermodynamic equilibrium). Exact quantum wave-packet reactive scattering calculations on a highly reliable potential energy surface for the $N(^2D) + H_2$ reaction using a highly accurate DMBE potential energy surface should also be highlighted. In relation with topic (b), we are performing quantum wave-packet calculations of reaction probabilities and cross sections for the prototypical $H + H_2^+$ reaction in its lowest triplet state potential energy surface including the GP effect, aiming to test whether a recently suggested[10] cancellation of such effects holds irrespective of the system. In (d), we have developed a Monte Carlo simulation method to calculate the classical partition function, and applied the technique to several prototypical systems. Semiempirical schemes to calculate quantum corrections to the classical partition function were also exploited with the results suggesting the method to be quite promising.

Research keywords: potential energy surfaces, electronic structure calculations, intermolecular forces, molecular dynamics, chemical dynamics, atmospheric ozone, ozone deficit problem, HO_x dilemma.

Research grants: Major continuing funding has been until 1992 by Instituto Nacional de Investigação Científica, and subsequently by Junta Nacional de Investigação Científica, and Fundação para a Ciência e a Tecnologia (Portugal). Many projects have been attributed ever since via this main route funding. They include since 1998:

- PRAXIS/C/QUI/10000/98: "Theory and computation of chemical reactions: from fundamental aspects to applications in environmental chemistry".

- POCTI/QUI/40154/2001: "Electronic structure and dynamics of reactive molecules: From fundamental issues to applications in environ-

[8] The index $\mathbf{v}$ denotes the three vibrational quantum numbers of the triatomic.

[9] For a review on our novel theory, see: D. Bradley, "Paradoxical Ozone", The Alchemist, January 14, 2004 (www.chemweb.com).

[10] "Theoretical study of geometric phase effects in the hydrogen-exchange reaction", J.C. Juannes-Marcos, S.C. Althorpe and E. Wrede, *Science* **309**, 1227 (2005).

mental chemistry, astrophysics and catalysis".

- POCI/QUI/60501/2004: "Quantum chemistry within the Born-Oppenheimer approximation and beyond: from first principles to predicting capability".
- POCI/AMB/60261/2004: "Theoretical Environmental Chemistry".
- REEQ/128/QUI/2005: "Computational chemistry with relevance in atmosphere, astrophysics and catalysis".
- PTDC/AAC-AMB/099737/2008: "Accurate theoretical studies on increasingly complex systems with environmental relevance".
- PTDC/QUI-QUI/099744/2008: "In pursuit of increasingly accurate molecular potentials and dynamics".

Other research funding has sporadically come from NATO, and Fundação Gulbenkian (Portugal). Collaborative research has also been funded via GRICES/Brazil-2004 ("Nonadiabatic theoretical chemical-physics: theory and application to simple systems and its isotopomers"), and GRICES/India-2007 ("Non-adiabatic interactions in molecular systems").

In 1994, the European Community funded a research project entitled "Multichannel Reactions and Combustion Modeling of Combustion Processes" presented to the Networks Activity of the Human Capital and Mobility Programme (Contract ERBCHRXCT940436). In 2002, the European Community approved a proposal (HPRN-CT-2002-00170) of a Research Training Network entitled "Predicting catalysis: Understanding ammonia production from first principles".

In 2008, the European Space Agency financed the proposal "Fundamental Issues in the Aerothermodynamics of Planetary Atmosphere Re-entry".

In 2011, Professor Donald G. Truhlar from the University of Minnesota, invited him for collaborative research on the Multidisciplinary Research Initiative (MURI) for Fundamental Processes in High-Temperature Hypersonic Flows under the auspices of the U.S. Air Force.

Lectures and communications

Posters

Presented numerous (over 250) poster communications in scientific

congresses.

Prize: First Prize for Best Poster in the "7th National Meeting of Physical Chemistry" of the Portuguese Chemical Society (Porto, Portugal, May 2005) with the work: *Theoretical Study of the* $O + ClO_2$ *reaction using an improved potential energy surface* by O.B.M. Teixeira, J.M.C. Marques and A.J.C. Varandas.

Lectures/seminars at Universities and research Institutes:
- University of Sussex (England)
- Universidade do Porto (Portugal)
- Instituto Superior Técnico (Portugal)
- Instituto de Física Matemática (Portugal)
- Universidade de Coimbra/Departamento de Física (Portugal)
- Universidad de Salamanca (Spain)
- Universita di Perugia (Italy)
- University of Minnesota (United States of America)
- National Argonne Laboratory (U.S.A.)
- Université de Reims-Societé Française de Chimie (France)
- Max-Planck-Institut für Strömungsforschung (Germany)
- Université de Bordeaux 1 (France)
- Universitat de Barcelona (Spain)
- University of Emory (U.S.A.)
- Jagiellonian University (Poland)
- Instituto Superior de Ciencias y Tecnologia Nuclear (La Habana, Cuba)
- Universidad Pedagógica "Rafael María de Mendive" (Pinar del Rio, Cuba)
- Universidade Federal do Rio de Janeiro (Brazil)
- Université de Pau et des Pays de l'Adour (France)
- Universidad Autonoma de Madrid (Spain)
- Universidad de Santiago de Compostela (Spain)
- Universidade de Minas Gerais/Departamento de Química (Brazil)
- Universidade de Brasília (Brazil)
- Facultad de Química, Universidad de La Habana (Cuba)
- Southwest Jiaotong University (Chengdu, China)
- Chengdu University at Dujiangyan (China)
- Universidad de La Habana/Facultad de Fíisica (La Habana, Cuba)
- University of New York/Department of Chemistry (U.S.A.)
- University of Nevada Las Vegas/Department of Chemistry (U.S.A.)
- University of Lund/Department of Chemistry (Sweeden)
- Universidade de Brasília/Departamento de Fíisica (Brazil)

- Universidade de Minas Gerais/Departamento de Fíisica (Brazil)
- Universidad de Matanzas/Departamento de Quimica (Cuba)
- Michigan State University/Department of Chemistry (U.S.A.)
- Dalian Institute of Chemical Physics/State Key Laboratory on Molecular Reaction Dynamics, (Dalian, China)
- Shandong Normal University/Department of Physics (Jinan, China)
- Shandong University/Department of Chemistry (Jinan, China)
- Dalian University of Technology/State Key Laboratory of Fine Chemicals, (Dalian, China)
- Dalian Marithime University/Department of Chemistry (Dalian, China)
- Northwest University/Department of Chemistry (Xian, China)
- Nanjing University/Department of Chemistry (Nanjing, China)
- Lianing Normal University/Department of Chemistry (Dalian, China)
- Henan Normal University/Department of Physics (Henan, China)
- Southwest Petroleum University/College of Chemistry & Chemical Engineering (Chengdu, China)
- Universidade de São Paulo/Instituto de Física (São Paulo, Brazil)
- Universidade Federal de Juiz de Fora/Departamento de Química (Juiz de Fora, Brazil)
- Faculdade de Ciências, Universidade de Lisboa (Portugal)
- Institute of Chemistry, Chinese Academy of Sciences (Beijing, China)
- IIT Kanpur, (Kanpur, India)
- IISER Mohali MGSIPAP Complex, (Chandigarh, India)
- Liaoning University, Department of Physics (Shenyang, China)
- East China Normal University, Department of Physics (Shangai, China)
- Indian Association for the Cultivation of Science, (Kolkata, India).
- Universidad Nacional Autonoma de Mexico, Instituto de Investigaciones en Materiales (Mexico City, Mexico.)
- Universidade Federal do Espírito Santo, Departamento de Física (Vitória, Brazil).
- University of Calcutta, Department of Chemistry, (Kolkata, India).

† Only cited at the occasion of first talk, roughly ordered by date of visit.

Major invited lectures and communications at congresses or seminar series:

1. "Two-body, atom-atom, and three-body, atom-atom-atom, interactions: strategy and use in spectroscopic and molecular dynamics calculations", *6º Encontro Anual da Sociedade Portuguesa de Química* (Aveiro, Portugal, 1983).

2. "A general approach to the potential energy surfaces of small polyatomic systems: molecules and van der Waals molecules", *XV Conferência dos Químicos Teóricos de Expressão Latina CHITEL* (Braga, Portugal, 1984).

3. "Intermolecular and intramolecular potentials: the general strategy of the double many-body expansion", *II Encuentro de Dinâmica Molecular* (Salamanca, Spain, 1986)

4. "Double many-body expansion of molecular potential energy functions and the role of long range forces in the rates of chemical reactions", *XVII CHITEL* (Peníscola, Spain, 1987).

5. "Non-central potentials for molecular dynamics", *XXI Reunion Bienal da Real Sociedad Española de Física* (Salamanca, Spain, 1987).

6. "The long range parts of potential energy surfaces and their role in the rates of chemical reactions", *I Congreso Nacional del Grupo Especializado de Física Atómica y Molecular* (Madrid, Spain, 1988).

7. "Química computacional: da estrutura à reactividade molecular", *Encontro de Física, Computação e Redes* (Coimbra, Portugal, 1988).

8. "The calculation and use of potential energy surfaces for molecular reaction dynamics and the role of long range forces", *NATO ASI on Computational and Theoretical Models for Organic Chemistry* (Vimeiro, Portugal, 1990); three lectures.

9. "The semiempirical double many-body expansion method for potential energy surfaces", 8^{th} *Seminar on Computational Methods in Quantum Chemistry* (Odense, Denmark, 1990).

10. "Funções de energia potencial e dinâmica das reacções", 7^{a} *Conferência Nacional de Física* (Lisboa, Portugal, 1990).

11. "Theoretical studies of long range forces in relation to the double many-body expansion method for potential functions and their role in reactivity", *XXIII Reunion Bienal da Sociedad Española de Química* (Salamanca, Spain, 1990).

12. "Recent progress on double many-body expansion potential energy surfaces for small polyatomics ($n \leq 4$) and their use for reactive scattering", *III Congreso National del Grupo Especializado de Física Atómica y Molecular* (Toledo, Spain, 1990).

13. "On the calculation and use of double many-body expansion potential energy surfaces in chemical reaction dynamics", *XIII International Symposium on Molecular Beams* (Madrid, Spain, 1991).

14. "Realistic molecular potential energy surfaces, the role of long range forces, and the double many-body expansion", *First International Conference on Atomic and Molecular Dynamics* (Taipei, Taiwan, 1991).

15. "Potential energy surfaces from quantum chemistry calculations", *1st EPS Southern European School of Physics "Dynamical Processes in Molecular Physics"* (Avila, Spain, 1991); three lectures.

16. "Estudo teórico de reacções químicas elementares: da energética à dinâmica", *Colóquio sobre Termodinâmica e Reactividade de Sistemas Moleculares* (Academia de Ciências de Lisboa, Portugal, 1991).

17. "On elementary chemical reactions", *13º Encontro Anual da Sociedade Portuguesa de Química* (Lisboa, Portugal, 1992); Lecture "Prémio Ferreira da Silva".

18. "On elementary chemical reactions: intermolecular and intramolecular forces acting together", *First South European Conference on Atomic and Molecular Physics* (Gandía-Valencia, Spain, 1992).

19. "Anisotropic long range forces, potential energy functions, and reaction rates", *NATO Advanced Research Workshop on Orientation and Polarization Effects in Chemical Reaction Dynamics* (Assisi, Italy, 1992).

20. "Potential energy surfaces, reaction dynamics, and zero-point energy problem in trajectory calculations", *First Congress of the International Society of Theoretical Chemical Physics* (Girona, Spain, 1993). Also member of pannel for discussion on "Reaction Dynamics".

21. "From global double many-body expansion potential energy surfaces to local modelling using gradients and hessians", *CCP6 Workshop on Fitting Molecular Potential Energy Surfaces* (Durham, England, 1993).

22. "Molecular potential energy functions" and "Quasiclassical trajectory methods and the problem of zero-point energy flow", *Summer School on Stereodynamics via Lasers and Molecular Beams* (Almería, Spain, 1994); two lectures.

23. "Reaction dynamics with and without global potential energy surfaces", *Tenth European Conference on the Dynamics of Molecular Collisions* (Salamanca, Spain, August 1994).

24. "Potential energy surfaces for studying the spectroscopy and dynamics of small polyatomic systems", *Workshop on Intramolecular Dynamics and Spectroscopy* (Telluride, Colorado, USA, July 1995).

25. "A double many-body expansion formalism for multivalued potential energy surfaces", *Workshop on Calculations of Potential Energy Functions* (Marne-la-Vallée, France, September 1995).

26. "Potential energy surfaces of reactive systems with relevance in combustion chemistry, including exploratory results for HOCN", *HCM Seminar on Multichannel Reactions and Kinetic Modeling* (Heidelberg, Germany, October 1995).

27. "A tale of two reactions: $H + O_2 + Ar$, an atmospheric reaction, $O_2(v') + O_2(v'')$, a reaction with implications in atmospheric ozone production", *HCM Seminar on Multichannel Reactions and Kinetic Modeling* (Bordeaux, France, May 1996).

28. "Theoretical studies of collisional dynamics: the atmospheric reactions $H + O_3$ and $O_2(v') + O_2(v'')$", *14th International Gas Kinetics Symposium* (Leeds, U.K., September 1996).

29. "Recent developments in potential energy surfaces", *XXIII Congreso Internacional de Quimicos Tepricos de Expresion Latina (QUITEL)* (Caceres, Spain, September 1996).

30. "On three-atom reactions and beyond", *3rd South European Conference on Atomic and Molecular Collisions* (Island of Kos, Greece, October 10-16, 1996).

31. "Current issues in molecular potential energy surfaces and dynamics: systems involving conical intersections", Symposium *Interactions of Oriented Molecules* (Bielefeld, Germany, June 30-July 3, 1997).

32. "Potential energy surfaces and dynamics of chemical reactions", *Second European Conference on Computational Chemistry: Present Achievements and Future Challenges* (Lisboa, Portugal, September 2-6, 1997).

33. "Potential-energy hypersurface modelling and chemical dynamics: the challenge of conical intersections", *John Murrell 65th Birthday Meeting* (Sussex, U.K., December 5, 1997).

34. "Current issues in potential energy surfaces and reaction dynamics", 7^{th} *Cuban School of Theoretical Chemistry* (La Habana, Cuba, January 6-16, 1998); three lectures.

35. "Classical and quantum dynamics studies of elementary chemical processes", *Symposium on Elementary Chemical Processes* (Perugia, Italy, July 10-13, 1998).

36. "Multivalued potential energy surfaces and the role of geometric phase effects in vibrational levels and resonances of reactive systems", *ECAMP VI Conference* (Siena, Italy, July 14-18, 1998).

37. "Advances and continuing challenges on potential energy surfaces and reaction dynamics", *XXIV Congreso Internacional de Químicos Teóricos de Expresión Latina* (H. Puebla de Z., Mexico, Sept 20-25, 1998).

38. "Diabolical conical intersections: modelling and role in molecular dynamics", *6me Réunion des Chimistes Théoreticiens Français* (Lile, France, October 13-16, 1998).

39. "Generalized Born-Oppenheimer calculations on systems involving conical intersections", *International Workshop on Current Issues in Structure and Molecular Dynamics* (Quilmes, Argentina, November 16-17, 1998).

40. "Quantum and classical studies of four-atom reactions, including novel elastic optimum angle adiabatic methods", *International Workshop on Current Issues in Structure and Molecular Dynamics* (Quilmes, Argentina, November 16-17, 1998).

41. "On the theoretical study of elementary reactions with relevance in environmental chemistry", *Congreso da Sociedad Cubana de Quimica* (La Habana, Cuba, December 1-3, 1998).

42. "Potential energy surfaces and quantum reduced-dimensionality *vs* classical calculations of four-atom chemical reactions", *Humbolt Symposium on Chemistry* (La Habana, Cuba, March 8-12, 1999).

43. "Conical intersections and their effect on molecular dynamics", *Fourth South European Conference on Atomic and Molecular Physics* (Gandía-Valencia, Spain, June 16-20, 1999). Also member of pannel for discussion on "Electronic structure calculations and reaction dynamics".

44. "Multivalued potential energy surfaces for dynamics calculations", *1st European Computational Chemistry School: Reaction and Molecular Dynamics* (Perugia, Italy, June 28-July 4, 1999).

45. "Current issues on potential energy surfaces and dynamics: the challenge of conical intersections", *The 1999 Dynamics of Molecular Collisions Conference* (Split Rock Resort in Lake Harmony, Pennsylvania, USA, July 18-23, 1999).

46. "On the geometrical phase and generalized Born-Oppenheimer calculations for systems involving conical intersections", *III Congress of the International Society for Theoretical Chemical Physics* (Mexico City, Mexico, November 8-13, 1999).

47. "Conical intersections: from topological aspects to implications in molecular dynamics", *X Simpáosio Brazileiro de Química Teórica* (Caxambu, Brazil, November 21-24, 1999).

48. "Generalized Born-Oppenheimer approximation: the geometric phase in $2D$ Hilbert space models", *Workshop on Photodynamics: From Isolated Molecules to Condensed Phases* (La Habana, Cuba, February 14-19, 2000).

49. "Generalized Born-Oppenheimer approximation and the geometric phase effect: dynamics in the vicinity of a crossing seam", *Fifth European Workshop on Quantum Systems in Chemistry and Physics* (Uppsala, Sweeden, April 13-18, 2000).

50. "Conical intersections and their topological effect on nuclear dynamics", *IV Iberian Meeting on Atomic and Molecular Physics* (El Escorial, Spain, May 30-June 2, 2000).

51. "Generalized Born-Oppenheimer treatment of systems with electronic degeneracies", *Chemical Dynamics at the Dawn of the Millenium*, Satelite Meeting of the X International Congress on Quantum Chemistry (Arcachon, France, May 31-June 3, 2000).

52. "Superficies de energia potencial: do conceito às aplicações", *VII Escola Brazileira de Estrutura Electráonica* (Goiânia, Brazil, July 16-20, 2000).

53. "Quantum dynamics in the vicinity of degeneracies: generalized Born-Oppenheimer treatment", *MOLEC 2000* (Jerusalem, Israel, September 17-22, 2000).

54. "Theoretical studies of bimolecular environmental reactions: Can the $OH + O_2$ reaction be a new source of stratospheric ozone?", *Stereodynamics 2000* (El Escorial, Madrid, Spain, December 1-5, 2000).

55. "Cyclic phases at N-fold Jahn-Teller degeneracies", *Workshop on Quantum Reaction Dynamics* (Caltech, Pasadena, California, USA, January 11-13, 2001).

56. "Theoretical & Computational Chemistry @ Coimbra", *Theoretical Chemistry Workshop of Tempus "TRUCS" Closing Seminar* (Krakow, Poland, February 22-24, 2001).

57. "Classical and quantum studies of stratospheric reactions: Is the HO_x cycle an ozone depleting one?", *The Second Informal Conference on Reaction Kinetics and Atmospheric Chemistry* (Helsingor, Denmark, June 8-10, 2001).

58. "The geometric phase effect: from mathematical modelling to applications in molecular dynamics", *ICTMA-10 (The 10th International Conference on the Teaching of Mathematical Modelling and Applications)* (Beijing, China, July 29-August 2, 2001).

59. "From energy landscapes to chemical kinetics", *5o Congresso de Química-Física da Sociedade Portuguesa de Química* (Faro, Portugal, September 12-14, 2001). Opening lecture.

60. "Strategies for global potential energy surfaces", *4th Seminars of Advanced Studies on Molecular Design and Bioinformatics* (La Habana, Cuba, February 3-9, 2002) (2 lectures).

61. "Theoretical reappraisal of the O_x and HO_x cycles in the high atmosphere", *Second International Meeting on Photodynamics* (La Habana, Cuba, February 10-16, 2002).

62. "Cyclic phases at Jahn-Teller degeneracies", *IV International Society for Theoretical Chemical Physics* (Marly-Le-Roi, Paris, July 9-16, 2002).

63. "Quest for ozone sources in the high atmosphere: theoretical reappraisal", *International Symposium on Frontiers in Molecular Science* (Qingdao, China, July 15-18, 2002).

64. "Current issues in non-adiabatic chemistry", *XXIV Congreso Internacional de Químicos Teóricos de Expresión Latina* (Montevideo, Uruguay, September 1-8, 2002). Opening lecture.

65. "Strategies for accurate global potential energy surfaces", *Predicting Catalysis: First Network Meeting* (Copenhagen, January 11-14, 2003).

66. "From single- to multi-sheeted potential energy surfaces: A dual strategy for accurate global representations", CCP1/CCP6 ChemReact Workshop on *High Accuracy Potentials for Quantum Dynamics* (London, March 31-April 2, 2003).

67. "From energy landscapes to dynamics of reactive species with relevance in the high atmosphere", *XX International Symposium on Molecular Beams* (Lisboa, June 8-13, 2003).

68. "Modelling and use in dynamics of electronic manifolds", *7th Workshop on Quantum Reactive Scattering* (El Escorial, Madrid, Spain, June 20-23, 2003).

69. "On the ro-vibrational spectroscopy of $H_3^+(^3A')$ ion and kinetics of HO_x ozone cycle", *Symposium in Memory of Professor Gert Due Billing* (Copenhagen, August 11-13, 2003).

70. "From trihydrogen insterstellar ion to hydrogen-oxygen reaction networks in terrestrial middle atmosphere", *I Congreso Nacional de Astroquímica* (Ciudad Real, Spain, December 1-4, 2003).

71. "Unraveling interstelar $H_3^+(^3A')$ and the paradoxical HO_x systems in the middle atmosphere", *Third International Meeting on Photodynamics* (La Habana, Cuba, February 16-20, 2004).

72. "Cyclic phases at electronic degeneracies", *Encontro Nacional da Física da Matéria Condensada* (Poços de Caldas, Minas Gerais, Brazil, May 4-8, 2004).

73. "Química teórica: una herramienta predictiva para la comprensión de los fenómenos de la atmósfera", *VI Taller Internacional Ecologia y Desarrollo (ECODES'04)* (Universidad de Matanzas, Cuba, June 4-8, 2004). Conferencia Magistral inaugural.

74. "From energetics to dynamics: Ro-vibrational spectroscopy of $H^+(^3A')$ and kinetics of reaction networks in atmospheric ozone chemistry", *DICP Symposium on Molecular Dynamics* (Dalian, China, July 21-23, 2004).

75. "Geometrical phases in Jahn-Teller systems and ro-vibrational spectroscopy of triplet-state trihydrogen ion", *CCP6 Workshop in Quantum Dynamics at Conical Intersections* (Nunspeet, The Netherlands, September 2-5, 2004).

76. "Global potential energy surfaces with near spectroscopic accuracy", *Computational Chemical Dynamics: from Gas-Phase to Condensed-Phase Systems* (Minneapolis, USA, October 7-9, 2004).

77. "Electronic manifolds and the geometrical phase effect in Jahn-Teller systems: Current developments and continuing challenges", *DAE-BRNS Symposium on Theoretical Chemistry* (Mumbai, India, December 9-12, 2004).

78. "Accurate global potential energy surfaces and ro-vibrational states of triatomic molecules", *American Physical Society March Meeting* (Los Angeles, California, U.S.A., March 21-25, 2005).

79. "Accurate global potential energy surfaces and dynamics calculations", *VIII Workshop on Quantum Reactive Scattering* (Santa Cruz, USA,July 15-19, 2005).

80. "General strategy for global potentials of near spectroscopic accuracy and geometrical phase implications in the rovibronic states of an X_3-type molecule", *1st International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry* (Yantai, China, May 22-24, 2005).

81. "Accurate global potentials and their topological implications in molecular dynamics", *XXXI Congreso Internacional de Químicos Teóricos de Expresión Latina* (Isla de Margarita, Venezuela, October 2-6, 2005).

82. "A general strategy for global potentials of near spectroscopic accuracy", *III Workshop em Física Molecular e Espectroscopia* (Belo Horizonte, Brazil, November 17-19, 2005).

83. "Accurate potentials and quantum dynamics of reactive molecules", *XIII Simpósio Brasileiro de Química Teórica* (Sï¿½o Pedro, Sï¿½o Paulo, Brazil, November 20-23, 2005).

84. "Reaction dynamics within the adiabatic approximation and beyond", *Fourth International Meeting on Photodynamics* (La Habana, Cuba, February 6-10, 2006).

85. "N_2H_2: an overview of the double-many body expansion method for potential energy surfaces, and how reliable is transition state theory", *Workshop "Predicting catalysis: from ammonia production to the hydrogen economy."* (Leiden, The Netherlands, June 21-23, 2006).

86. "Prediction by scaling of the electron correlation and use in dynamics of global potential energy surfaces", *Chinese Academy of Sciences Symposium on Computational Chemistry and Parallel Software" (CAS-SCCPS* (Zhangjiajie, China, July 10-12, 2006).

87. "Molecular reaction dynamics within the adiabatic approximation and beyond", *Mathematics in Chemistry: A CIM Workshop* (Lisboa, Portugal, July 19-21, 2006).

88. "From electron-correlation scaling to accurate potential energy surfaces", *European Symposium Series "Quantum Systems in Chemistry and Physics", QSCP-XI* (S. Petersburg, Russia, August 20-25, 2006).

89. "Prediction by scaling of the electron correlation and modeling of highly accurate global potential energy surfaces", *MOLEC 2006 - European Conference on Dynamics of Molecular Systems"* (Levico Terme, Trento, Italy, September 11-15, 2006).

90. "From molecular potentials to dynamics within the Born-Oppenheimer approximation and beyond", *Meeting of the Born-Oppenhei-mer Working Group*, (ESTEC, Nordwijk, The Netherlands, May 14, 2007).

91. "Accurate ab initio potential energy surfaces: Can they be obtained at low cost?", *20th International Conference on Molecular Energy Transfer* (Arcachon, France, June 3-7, 2007).

92. "Environmental chemistry: a molecular perspective", *VIII Taller Internacional Ecologia y Desarrollo (ECODES'07)* (Matanzas, Cuba, June 12-15, 2007).

93. "Highly accurate molecular potential energy surfaces: calculation and use in dynamics", *IX Workshop on Quantum Reactive Scattering* (Cambridge, U.K. July 18-22, 2007).

94. "Highly accurate molecular potential energy surfaces via conventional ab initio methods: calculation and use in dynamics", *European Symposium Series "Quantum Systems in Chemistry and Physics", QSCP-XII* (London, Royal Holloway, University of London, UK, August 30-September 5, 2007).

95. "Da estrutura e dinâmica das moléculas 80 anos após a aproximaçäo de Born-Oppenheimer", Academia das Ciências de Lisboa (Lisboa, October 4, 2007).

96. "Sobre moléculas e colisões moleculares: uma perspectiva teórica", Ciclo de Seminários Professora Marieta da Silveira - DQB 2007/2008, Faculdade de Ciências da Universidade de Lisboa (Lisboa, January 9, 2008).

97. "Molecular potentials and dynamics. beyond a single electronic state", Fundamental Issues in the Aerothermodynamics of Planetary Atmosphere Re-entry (ULB, Brussels, February 14, 2008).

98. "Accurate molecular potentials by conventional ab initio methods", *13th International Workshop "Quantum Systems in Chemistry and Physics" (QSCP-XIII)*, Lansing, Michigan, USA, July 6-12, 2008.

99. "Scaling and extrapolation of ab initio molecular energies: clues to highly accurate potentials for use in dynamics", *6th ESPA (Electronic Structure: Principles and Applications)* Palma de Mallorca (Balearic Islands, Spain, September 2-5, 2008).

100. "Accurate potential energy surfaces and dynamics: Clues for a cost-effective general strategy", *8th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC)* Sydney (Australia, September 14-19, 2008).

101. "Toward high-accuracy *ab initio* potentials at low cost", *International Conference on Theory and Applications of Computational Chemistry (TACC)* Shangai (China, September 23-27, 2008).

102. "In pursuit of high-accuracy ab initio potentials for spectroscopy and reaction dynamics", *TCS Discussion Meeting on Theoretical Chemistry* Bangalore (India, January 19-23, 2009).

103. "Eight decades of Born-Oppenheimer approximation", *Endowment lecture at Raman Center for Atomic, Molecular and Optical Sciences* Kolkata (India, January 27, 2009).

104. "*Ab initio* methods for accurate potential energy surface calculations: the triatomic systems N_3, NO_2 and H_3^+", *First Progress Meeting, European Space Agency* (IST, Lisboa, May 25, 2009).

105. "In pursuit of a cost-effective strategy for accurate *ab initio* potential energy surfaces in reaction dynamics", *10th International Quantum Reactive Scattering (QRS) Workshop* Dalian (China, June 6-10, 2009).

106. "Recent progress on global potential energy surfaces: an ab initio cost-effective strategy", *14th International Workshop "Quantum Systems in Chemistry and Physics" (QSCP-XIII)*, to be held El Escorial, Madrid, Spain, September 13-19, 2008.

107. "Accurate adiabatic and diabatic ab initio potentials, and their use in molecular reaction dynamics", *XXXV QUITEL (Congress of Theoretical Chemists of Latin Expression)* (San Andres Island, Colombia, September 18-22, 2009).

108. "Adiabatic approximation and its topological implications", *Second Progress Meeting, European Space Agency* (UCL, London, November 9-10, 2009).

109. "Adiabatic approximation and the appearance of geometrical phases at diabolic intersections" *Quantal aspects in Chemistry & Physics (Tribute to the memory of Ruy Couceiro da Costa)* (Academia das Ciências de Lisboa, Portugal, Novembro 27, 2009).

110. "To be announced", *Seventh International Meeting on Photodynamics* (La Habana, Cuba, February 1-5, 2010).

111. "Non-adiabatic potential energy surfaces for triatomic systems", *Third Progress Meeting* (Engineering Faculty, University of Rome "LaSapienza, Rome, Italy, May 28, 2010).

112. "Cyclic phases in Jahn-Teller systems", *XXth International Symposium on the Jahn-Teller Effect* (Fribourg, Swizerland, August 16-20, 2010).

113. "Toward a global multisheeted potential energy surface for the $NO_2(^2A'')$ electronic manifold", *XXth International Symposium on the Jahn-Teller Effect* (Fribourg, Swizerland, August 16-20, 2010); authored by V.C. Mota, P.J.S.B. Caridade and A.J.C. Varandas, communicated by V.C. Mota.

114. "Quantum mechanical study of the $S(^1D)+H_2$ reaction and its isotopic variants", *MOLEC XVIII* (Curia, Portugal, September 5-10, 2010); authored by M. Hankel, S.C. Smith, H. Yang, K.-L. Han, G.C. Schatz and A.J.C. Varandas, communicated by M. Hankel.

115. "$S(^1D)+H_2$ reaction dynamics at very low collision energies", *MOLEC XVIII* (Curia, Portugal, September 5-10, 2010); in authored by M. Lara, P.G. Jambrina, F. Dayou, J.-M. Launay, A.J.C. Varandas and F.J. Aoiz, communicated by M. Lara.

116. "*Ab initio*-based molecular potentials and their topological implications in dynamics", *CHITEL 2010*, (Anglet, France, September 19-24, 2010).

117. "Toward a global multisheeted potential energy surface for the first three $^2A''$ states of NO_2", *CHITEL 2010*, (Anglet, France, September 19-24, 2010); authored by V.C. Mota, P.J.S.B. Caridade and A.J.C. Varandas, communicated by V.C. Mota.

118. "Ab-initio-based electronic manifolds and reaction dynamics", *Theoretical Chemistry Symposium (TCS10)* (Indian Institute of Technology, Kanpur, India, December 8-12, 2010).

119. "Topological phases and dynamics at conical intersections", *Endowment lecture at Indian Association for the Cultivation of Science*, Kolkata (India, December 20, 2010).

120. "*Ab initio*-based potentials and dynamics with relevance in environmental chemistry", *Chemical Physics of Low Temperature Plasmas* (Bari, Italy, January 31-February 1, 2011).

121. "*Unraveling the isomerization and rupture of the elusive* HO_3 *radical*", *XXIV International Symposium on Molecular Beams* (Bordeaux, France, May 23-26, 2011).

122. "A tale of two issues: 1) HO_3 isomerization and rupture, 2) Dynamics of Jahn-Teller electronic manifolds", *8th Seminars of Advanced Studies on Molecular Design and Bioinformatics: Light and Molecules (SEADIM 8)* (La Habana and Varadero, July 10-15, 2011).

123. "Electronic structure and dynamics within the Born-Oppenheimer approximation and beyond", *11th International Workshop on Quantum Reactive Scattering (QRSC11)* (Santa Fe, New Mexico, July 17-21, 2011).

124. "Two quests: Weakness of HO_3, and Jahn-Teller dynamics via a generalized Born-Oppenheimer theory", *World Association of Theoretical and Computational Chemists (WATOC)* (Santiago de Compostela, Spain, July 17-22, 2011).

125. "Is there a fingerprint for onset of hydrogen-bonding in a chemical reaction? The elusive HO_3 radical", *XIX. International Conference on "Horizons in Hydrogen Bond Research"* (Göttingen, Germany, September 11-17, 2011).

126. "Accurate course of HO_3 dissociation, and beyond", *Spectroscopy and dynamics of ozone and related atmospheric species* (Reims, France, October 3-5, 2011).

127. "Odd-hydrogen: energetics and role on bimolecular and water-cluster mediated atmospheric reactions", *CIUM* (Varadero, Cuba, November 7-11, 2011).

128. "Recent progress on accurate *ab initio*-based potentials and dynamics: atmospheric N_xOy triatomic systems and beyond", *European Conference on the Atomic and Molecular Physics of Ionized Gases (ESCAMPIG XXI)* (Viana do Castelo, Portugal, July 10-14, 2012).

129. "From accurate molecular potentials to dynamics tumbling on crossings", *7th International Meeting on Photodynamics and Related Aspects* (Maresias, São Paulo, Brazil, October 14-20, 2012).

130. "Ozone depletion through the $HO_2 + nH_2O + O_3$ reaction: *ab initio* and KS-DFT studies", *XXXVIII Quitel* (Natal, Brazil, December 2-7, 2012), communicated by L.P. Viegas.

131. "Molecular potential energy surfaces and reaction dynamics", *XXXVIII Quitel* (Natal, Brazil, December 2-7, 2012).

132. "From molecular potentials to dynamics including conical seams', *Electronic Structure and Dynamics of Molecules and Clusters (ESDMC)* (Kolkata, India, February 17-20, 2013).

133. "De Schrödinger a Arrhenius na aproximação de Born-Oppenheimer e para além desta" (Departamento de Química, Universidade de Coimbra, April 3, 2013).

134. "From elementary reactions to the role of water in HO_x atmospheric chemistry: Just a catalyst or far beyond?", *International Symposium on Organic Reaction Mechanism -A celebration in honor of Bob Grubbs, Ken Houk, Paul Schleyer and Don Truhlar* (Peking University, Shenzhen, R.P. China, May 8-9, 2013).

135. "Recent developments in molecular potentials and reaction dynamics", *12th Workshop in Quantum Reactive Scattering* (Bordeaux, France, June 10 - 14, 2013).

136. "From accurate potentials and code for three-body quantum reactive scattering in hyperspherical coordinates to the dual role of water in HO_x atmospheric chemistry", *XXXIX Congreso Internacional de Químicos Teóricos de Expresión Latina - CHITEL* (Granada, Spain, June 30 - July 5, 2013).

137. "Accurate potentials and dynamics: the paradigmatic HO_x radicals and dual role of water in mediating reaction", *SEADIM 9: 9th Seminars of Advanced Studies on Molecular Design and Bioinformatics: Energy* (Varadero, Cuba, July 7 - 9, 2013).

138. "Title to be specified", *Quantum Systems in Chemistry and Physics)* (Paraty, Rio de Janeiro, Brasil, December 1 - 7, 2013).

139. "Title to be specified", *8th International Meeting on Photodynamics and Related Aspects* (Oaxaca, Mexico, October 2014).

Colloquial discussions

Participated on the first session of the cycle of discussions "Ao fio da conversa" entitled "Ciência e Cultura" organized by "Instituto de Investigaçäo Interdisciplinar" (Coimbra, November 21, 2002).

Awards

1985: "Artur Malheiros" Prize for Physics and Chemistry of

Lisbon Academy of Sciences.

1991: "Ferreira da Silva" Prize of Portuguese Chemical Society.

2004: Prize Stimulus to Excellence of the Portuguese Ministry of Science, Innovation and High Studies.

2009: "Rajendralal Mitra Endowment Lecture", Indian Association for the Cultivation of Science" (January 27, Kolkata, India).

2009: "Visiting Professor for Senior International Scientists" of the Chinese Academy of Sciences.

2010: "First Sadhan Basu Memorial Lecture", Indian Association for the Cultivation of Science" (December 20, Kolkata, India).

Other recognitions

2011: "Recognition for support and consciencitious supervision" by China Scholarship Council on the occasion of granting the "2010 Chinese Government Award for Outstanding Self-financed Chinese Students Study Abroad (January 24).

ISI's 10858 Most Cited Chemists, 1981-June 1997

Rank by total citations: 2890 (*top* 0.46 %).

ISI Web of Knowledge, 2005

Rank by total number of papers: 1830 (*top* 0.30 %).
Rank by total citations: 3167 (*top* 0.50 %).
Rank by total citations per paper: 4890 (*top* 0.78 %).

ISI Web of Knowledge, 2013

Sum of total citations: 6100.
Citing articles: 2603.
h-factor (May 2013): 42.

Not all papers appear as they should in ISI due to problems that have only to do with the Journal and Thompson-Reuters policies.

Appointments

Chemistry Department:

1989-92: Head of Department

1992-95: Chairman of Scientific Committee.

Other:

1979-81: Sociedade Portuguesa de Química-Delegação de Coimbra

(Zona Centro), chairman.

1981-92: Sociedade Portuguesa de Química-Delegação de Coimbra (Zona Centro), head of executive committee.

1985-89: Sociedade Portuguesa de Química, vice-president.

1987-89: Chemical Physics Division of European Physical Society, coopted member of board.

1989-95: Chemical Physics Division of European Physical Society, member of board.

1989-95: Fundação para o Desenvolvimento dos Meios Nacionais de Cálculo Científico - FCCN, university representative.

1989-92: Universidade de Coimbra, member of Senate.

1992- : International Society for Theoretical Chemical Physics, national representative.

1992-93: Committtee for Scientific Computation (Universidade de Coimbra), chairman.

Journals

Editorship:

1985-92 : Editor of Revista Portuguesa de Química.

Advisory editorial boards and/or Guest Editorships:

1997- : Asian Journal of Spectroscopy (Spectral-Force Publications, quarterly, India).

1999-2003: International Journal of Quantum Chemistry.

2000- : International Journal of Molecular Sciences (Switzerland).

2001-2003: PhysChemComm (UK's Royal Society of Chemistry).

2001- : Journal of Theoretical and Computational Chemistry (World Scientific Publishing).

2002- : Electronic Journal of Mathematical and Physical Sciences (www.EJMAPS.org).

2005- : International Journal of Applied Chemistry (IJAC, quarterly, Egypt).

2007- : The Open Chemical Physics Journal (Bentham Science's Journals, http://www.bentham.org/).

2012- : ISRN Physical Chemistry (International Scholarly Research Network, www.isrn.com/journals/physchem/).

2012- : The SciTech (The SciTech Publishers, India).

2012- : Dataset Papers in Chemistry (Datasets International, USA).

2012- : Computation (MDPI online, quarterly, Switzerland).

2012- : Communications in Computational Chemistry (Global Science Press, China).

2012- : International Journal of Chemoinformatics and Chemical Engineering (IJCCE).

2012- : Conference Papers in Chemistry (Hindawi Publishing Corporation).
2012- : AOCSR-Research Journal of Chemical Sciences.

International meeting MOLEC:

2000- : Member of the International Scientific Committee of MOLEC (European Conference on the Dynamics of Molecular Collisions).

Other meetings and festivals

1980: *3º Encontro Anual da Sociedade Portuguesa de Química* (Coimbra), Chairman.
1982: *4º Encontro Anual da Sociedade Portuguesa de Química* (Porto), Organizing Committee.
1982: *Symposium on Molecular Forces and Molecular Dynamics* (Coimbra), scientific and organizing committees.
1983: *6º Encontro Anual da Sociedade Portuguesa de Química* (Coimbra and Aveiro), Coordinating Committee.
1986: *9º Encontro Anual da Sociedade Portuguesa de Química* (Coimbra), Chairman of Scientific Committee.
1987: *10º Encontro Anual da Sociedade Portuguesa de Química* (Porto), Scientific Committtee.
1988: *Third Europhysics Summer School on Chemical Physics* (Santander, Spain), Organizing Committee.
1989: *Symposium on Applied Theoretical Chemistry* at *European Conference on Atomic and Molecular Physics* (Bordeaux, France), Organizing Committee.
1990: *Computadores no Ensino da Física e da Química* (Coimbra), Scientific Committee.
1991: *12º Encontro Anual da Sociedade Portuguesa de Química* (Coimbra), Scientific Committee.
1993: *Seminar on Supercomputers and Chemical Reactivity* (Coimbra), Head.
1994: *2nd South European Conference on Atomic and Molecular Physics* (Pisa, Italy; September 27-30), Scientific Committee.
1995: *Second Iberian Joint Meeting on Atomic and Molecular Physics* (Bilbao, Spain; July 10-12), Scientific Committee.
1997: *HCM Meeting on Multichannel Reactions and Kinetics Modelling of Combustion Processes* (Coimbra, March 21-22

1997), Head.

1998: *Third Iberian Joint Meeting on Atomic and Molecular Physics* (Mira, Portugal, May 4-7), Scientific and Organizing committees.

1998: *XXIV Congreso Internacional de Químicos Teóricos de Expresión Latina* (H. Puebla de Z., Mexico, September 20-25), Scientific Committee.

1999: *Ciclo de Lições em Química Teórica* (Coimbra, January 27-February 8), Head.

1999: *FILMOBIDOS'99 - II Festival Internacional do Filme Médico e Científico* (Óbidos, Portugal, May 18-22), International Scientific Committee.

2000: *Photodynamics from Isolated Molecules to Condensed Phases* (La Habana, Cuba, February 13-19), International Advisory Board.

2001: *FILMOBIDOS' 2001*, (Óbidos, Portugal, May 22-26) International Evaluation Panel.

2001: *XXVII Congrés des Chimistes Théoriciens d'Expression Latine (CHITEL)* (Toulouse, France, September 3-7), International Scientific Committee.

2002: *Second Internation Meeting on Photodynamics* (La Habana, Cuba, February 10-16), International Advisory Board.

2002: *Fifth Iberian Joint Meeting on Atomic and Molecular Physics* (Lisboa, March 16-19), Scientific Committee.

2003: *XX International Symposium on Molecular Beams* (Lisboa, Portugal, June 8-15 2003), Scientific Committee.

2003: *Six Iberian Joint Meeting on Atomic and Molecular Physics* (Spain, July 9-10), Scientific Committee.

2003: *6º Encontro Nacional de Química-Física* (Lisboa, Portugal, August 31-September 3), Scientific Committee.

2004: *Third International Meeting in Photodynamics* (La Habana, Cuba, February 16-20), International Advisory Board.

2004: *EC Meeting on Predicting Catalysis: Understanding Ammonia Production from First Principles* (Coimbra, Portugal, April 23-25), Head.

2004 *XXX Congresso Internacional de Químicos Teóricos de Expressión Latina* (Porto, Portugal, September 8-12), Scientific Committee.

2006: *Fourth International Meeting in Photodynamics*
(La Habana, Cuba, February 6-10), International Advisory Board.

2006 *Mathematics in Chemistry: A CIM Workshop*
(Lisboa, Portugal, July 17-19), Scientific Committee.

2008: *Fifth International Meeting in Photodynamics*
(La Habana, Cuba, February 3-8), International Advisory Board.

2008 *QUITEL08 - XXXIV Congresso dei Chimici Teorici di Espressione Latina*, (Cetraro CS, Italia, July 3-8, 2008), Scientific Committee.

2009 *Encontro de Química-Física da Sociedade Portuguesa de Química* (Aveiro, June), Scientific Committee.

2009 *Aspectos Quânticos em Física e Química* (Conferência dedicada á Memória de Ruy Couceiro da Costa) (Academia das Ciências de Lisboa, Portugal, November 27, Organizing Committee.

2010 *ECAMP*-European Conference in Atomic and Molecular Physics (Salamanca, Spain, July), Scientific Committee.

2010 *MOLEC 2010*-European Conference on the Dynamics of Molecular Collisions (Portugal, Curia, September 5-10), Scientific Committee, Conference Chair.

2012 *International Meeting on Photodynamics and Related Aspects* (Maresias, S. Paulo, Brazil, October 14-20). Scientific Committee.

2013 *Electronic Structure and Dynamics of Molecule and Clusters (ESDMC)* (Kolkata, India, February 17-20). Organizing Scientific Committee.

Professional societies

Royal Society of Chemistry (U.K.)
European Physical Society
American Physical Society (U.S.A.)
American Chemical Society (U.S.A.)
International Society for Theoretical Chemical Physics
Sociedade Portuguesa de Física (Portugal)
Sociedade Portuguesa de Química (Portugal)
New York Academy of Sciences (U.S.A.)
Quantum Chemistry Program Exchange (U.S.A.)
International Association of Scientists in the Interdisciplinary Areas (IASIA) (Canada), Board of Advisors.

Invited Refereeing:

Journal of Physical Chemistry
Journal of Physical Chemistry *A*

Journal of Chemical Physics
Journal of the Chemical Society Faraday Transactions
Physical Chemistry Chemical Physics
Chemical Physics
Chemical Physics Letters
International Journal of Quantum Chemistry
Journal of the American Chemical Society
Asian Journal of Spectroscopy
Perkin Transactions
Zeitschrift für Physik D: Atoms, Molecules and Clusters
Journal of Molecular Structure THEOCHEM
Physics Letters A
Revista Portuguesa de Química
Theoretical Chemistry Accounts
Journal of Physics B: Atomic, Molecular & Optical Physics
ChemPhysChem
Journal of Computational Methods in Sciences and Engineering
Journal of Computational Chemistry
Surface Science
Journal Brazilian Chemical Society
Journal of Theoretical & Computational Chemistry
European Physics Journal D
Journal of Quantitative Spectroscopy and Radiative Transfer
Canadian Journal of Physics
Computational Materials Science
Journal of Molecular Modeling
Chinese Physics B (Institute of Physics, CAS)
RSC Advances (Royal Society of Chemistry)

Evaluation panels:

2005- Foreign expert of The Ministery of Research and New Techniques, France.

2010- ISCRA (Italian SuperComputing Resource Allocation) reviewer, Italian SuperComputing Resource Allocation promoted by, CINECA, Bologna, Italy.

Occasionally solicited for reviewing research proposals to:
National Science Foundation (NSF), USA;

Chinese Academy of Sciences, P.R. China.
State Natural Science Award of the People's Republic of China.
Council of Scientific & Industrial Research, India.

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3. *The calculation of dynamic polarizabilities and long-range dispersion energy coefficients*
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4. *On the calculation of the relativistic long-range coefficient* W_4
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5. *Perturbation calculations of rare-gas potentials near the van der Waals minimum*
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6. *Potential energy surface for the lowest quartet state of* H_3
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   Molec. Phys. **31**, 1129-1135 (1976)
7. *Analytical potentials for triatomic molecules from spectroscopic data. II. Application to ozone*
   J.N. Murrell, K.S. Sorbie and A.J.C. Varandas
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8. *A many-body expansion of polyatomic potential energy surfaces: application to* H_n *systems*
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12. *Chercher le croisement*
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13. *A LEPS potential for* H_3 *from force field data*
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14. *Hybrid potential function for bound diatomic- molecules*
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15. *Zeroth-order exchange energy as a criterion for optimized atomic basis sets in interatomic force calculations. Application to* He_2
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    Chem. Phys. Lett. **69**, 222-224 (1980)

16. *On the isotropic and leading anisotropic terms of the* $H-H_2$ *potential energy surface*
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17. *The use of vicinal* $H-H$ *coupling constants in rotational isomerism studies - I*
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20. *Diffusion coefficients of hydrogen atoms and molecules from accurate spherically averaged* $H - H_2$ *interaction potentials*
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