

## **CURRICULUM VITAE**

**Name:** Luis Alberto Montero-Cabrera

*Place of birth:* Havana, Cuba

*Date of birth:* January 2, 1947

*Gender:* Male

*Affiliation and mailing address:* Universidad de La Habana, Facultad de Química, La Habana 10400, Cuba

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*Citizenship:* Cuban

*IDN:* 47010200982

*Passport:* I175946, issued in Havana, 28/10/2013; expires 28/10/2019

*Status:* Married

*Present position:* Full Professor (Profesor titular), Full Researcher (Investigador titular)

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Hirsch index (Google Scholar, 01/09/2016; <https://scholar.google.com/citations?user=ZZlpOQwAAAAJ&hl=en>): 18

Researchgate index (01/09/2016; [https://www.researchgate.net/profile/Luis\\_Montero](https://www.researchgate.net/profile/Luis_Montero)): 36.53



### **General Education:**

- Columbus School, Havana, 1950-52
- Colegio De La Salle (Vedado), Havana, 1952-61
- Instituto Preuniversitario de La Habana "José Martí", Havana, 1962-63

### **Higher and Postgraduate Education:**

- Universidad de La Habana, Facultad de Ciencias, 1963-68, Licenciado en Química. Thesis: "*Espectros electrónicos de compuestos furánicos en soluciones diluidas congeladas*", with Y.I. Kozlov, Karpov Institute of Physical Chemistry (Moscow) - Instituto Cubano de Investigaciones sobre los Derivados de la Caña de Azúcar (La Habana).
- Technische Universität Dresden, Dresden, Germany, 1978-80, Dr. rer. nat. Thesis: "*Unified Approach to the Orbital Resonance Integrals in the Zero Differential Overlap Molecular Orbital Approximation*" with J. Fabian.
- Universidad de La Habana, 2012, Doctor in Sciences, Thesis: "*Imaginación asistida del nanomundo desde Cuba*"

### **Special and Graduate Education:**

- Spectroscopy and Physical Methods in Chemistry, Prof. V. Mastryukov, Universidad de La Habana, Havana, 1966
- French Language, Escuela "Abraham Lincoln", Havana, 1967-71
- Spectroscopic Methods for Natural Products, Prof. J. Elguero, et al., National Center for Scientific Research (CNIC), Havana, 1969 (by French lecturers)
- Quantum Chemistry, Profs. J. Fabian, A. Mehlhorn, CNIC, Havana, 1970 (by lecturers from Germany)
- Linear Algebra, Prof. A. González, CNIC, Havana, 1969-70
- Quantum Mechanics, Prof. E. Entrialgo, Universidad de La Habana, Havana, 1971 (undergraduate course for physicists)
- Advanced English Language, Prof. M. Moore, CNIC, Havana, 1974
- Marxist Philosophy, Prof. G.J. García Galló, CNIC, Havana, 1974-75
- German Language, Escuela "Ramos Latour", Universidad de La Habana, Havana, 1986-88

### **Awards:**

- *The Best Graduate in Sciences, Havana, 1968*
- *Medal for Teaching to Illiterates in 1961, Havana, 1986*
- *Medal "Rafael María de Mendive" for 25 Years in Education, Havana, 1989*
- *Medal to Cuban Education, Havana, 1991*
- *Medal "José Tey" for performance in Cuban education, Havana, 1995*
- *Outstanding work in the 11<sup>th</sup> National Forum for Science and Technology, Havana, 1996.*
- *Award to the best work applied to Higher Education in 1996, Universidad de La Habana, Havana, 1997.*
- *Award to the best work applied to Higher Education in 1996, Ministry of Higher Education of Cuba, Havana, 1997.*
- *"Outstanding Worker" in 1996 of the National Trade Union of Scientific Workers, Havana, 1997.*
- *"Outstanding Worker" in 1997 of the National Trade Union of Education, Havana, 1998.*
- *Award of the Ministry of Higher Education in 1997, Ministry of Higher Education of Cuba, Havana, 1997.*
- *Prize of the Academy of Sciences of Cuba in 1997 for a work on programs of computational chemistry in personal computers, Havana, 1998.*
- *Medal for the 270<sup>th</sup> Anniversary of the University of Havana, Havana, 1998.*
- *Honor Degree "Carlos J. Finlay" for Science, Council of State, Havana, 1999.*
- *"Outstanding Worker" in 1998 of the National Trade Union of Scientific Workers, Havana, 1999.*
- *"Outstanding Worker" in 1999 of the National Trade Union of Education, Havana, 2000.*
- *Prize of the Academy of Sciences of Cuba in 2000 for a work on computational simulations of zeolites (shared), Havana, 2001.*
- *Honor Degree "Frank Pais" (2nd. Degree) for Education, Council of State, Havana, 2000.*
- *Medal for Labor Deed, Council of State, Havana, 2002.*
- *Prize of the Academy of Sciences of Cuba in 2005 for a work on theoretical modeling of flavonoids (shared), Havana, 2006.*
- *"Premio Anual de la Salud" to the scientific article, Ministerio de Salud Pública, Havana, 2006*
- *Medal for the 280th Anniversary of the University of Havana, Havana, 2008.*
- *Award to the best results in the University of Havana on International Postgraduate Education in 2007-09, Havana, 2008.*
- *Award to the best results in Postgraduate Education in 2007-09, Ministry of Higher Education of Cuba, Havana, 2009.*
- *Distinción Universidad de La Habana por el Conjunto de la Obra Científica, Havana, 2009*
- *Selected among the "Educadores Destacados del Siglo XX" by the Asociación de Pedagogos de Cuba, Havana, 2009.*
- *Prize of the Academy of Sciences of Cuba in 2011 on "Modelación Teórica de Brasinoesteroides y sus Análogos", with Dr. Cercis Morera Boado, coauthor, Havana, 2012.*
- *Honor Degree "Frank Pais" (1st. Degree) for Education, Council of State, Havana, 2012.*
- *Prize of the Academy of Sciences of Cuba in 2012 on "Modelación computacional de absorción de luz por sistemas nanoscópicos", with Dr. Ana Lilian Montero Alejo, coauthor, Havana, 2013.*
- *Special Prize for Scientific Relevance of the Cuban Ministry of Science, Technology and Environment, coauthor, Havana, 2013.*
- *Profesor Tiza de Oro, Federación Estudiantil Universitaria, Facultad de Química, Universidad de La Habana, Havana, 2013*
- *Award for Dr. Sc. Thesis Dissertation, National Commission of Scientific Degrees, Havana, 2014.*
- *Emeritus Professor, Universidad de La Habana, Havana, 2015*
- *Honorary President, Sociedad Cubana de Química, Havana, 2018*

### **Scientific Research and Higher Education Teaching Themes:**

- *Cellulose Derivative Preparations (research), 1966-67, Universidad de La Habana-Instituto Cubano de Investigaciones sobre los Derivados de la Caña de Azúcar, dir: Jorge Lodos.*

- *Photophysics and Photochemistry of Organic Molecules* (research), 1967-72, Universidad de la Habana-Centro Nacional de Investigaciones Científicas, dir: Yuri Kozlov, Egon Fanghänel, Luis Montero.
- *Molecular Spectroscopy* (teaching and research), 1969-1979, Universidad de la Habana-Centro Nacional de Investigaciones Científicas, dir: Luis Montero.
- *Theoretical Chemistry* (teaching and research), 1970-, Centro Nacional de Investigaciones Científicas-Universidad de La Habana-Academia de Ciencias de Cuba, dir: Luis Montero.
- *Applications of Molecular Modeling to Biological Problems and Theoretical QSAR* (research), 1981-, Academia de Ciencias de Cuba - Universidad de La Habana, dir: Luis Montero.
- *Science Policy* (research), 1970-1982, Ministerios de Educación y de Educación Superior, dir.: Luis Montero.
- *Statistical Thermodynamics* (teaching), 1979-1992, Universidad de La Habana.
- *Quantum Chemistry* (teaching and research), 1982-, Universidad de La Habana.
- *Computer Sciences* (teaching), 1986-, Universidad de La Habana.
- *FORTRAN and BASIC programming* (teaching and research), 1970-, Universidad de La Habana-Centro Nacional de Investigaciones Científicas, dir: Luis Montero.
- *Linux operating system* (teaching and research on applications), 1994-, Universidad de La Habana, dir. Luis Montero
- *Bioinformatics: molecular modeling of biological processes*, 2001 -, Universidad de La Habana, dir. Luis Montero.
- *Science Policy*, 1972 -, Universidad de La Habana, dir. Luis Montero

**Important scientific languages:**

(Regular=R, Good=G, Correct=C)

	<i>Speaking</i>	<i>Reading</i>	<i>Writing</i>
Spanish	C	C	C
English	C	C	C
French	G	C	R
German	R	R	R

**Guided Doctorate Degrees:**

1. Dr. Chemical Sciences, **Juan Raúl Álvarez - Idaboy**, *Theoretical Model of Electrophilic Substitution in Furan Compounds*, Universidad de La Habana, Facultad de Química, La Habana, Cuba, 1991.
2. Dr. Chemical Sciences, **Luis René Sierra - Medina**, *Theoretical Model of Zeolite Structure and Reactions*, Universidad de La Habana, Facultad de Química, La Habana, Cuba, 1995.
3. Dr. Physical Sciences, **Mario Piris - Silvera**, *An Application of the Bardeen - Cooper - Schrieffer Approach to Electron Correlation in Molecules*, Center for Nuclear Applications and Development, La Habana, Cuba, 1997.
4. Dr. Chemical Sciences, **Ernesto Estrada - Roger**, *Study about New Graph-Theoretical Models for Molecular Design in Organic Chemistry*, Universidad Central de Las Villas, Centro de Bioactivos Químicos, Santa Clara, Cuba, 1997.
5. Dr. Physical Sciences, **Ángel Rabel Ruiz - Salvador**, *Methodologies for Computational Studies of Zeolites*, Instituto de Materiales y Reactivos, La Habana, Cuba, 1999.
6. Dr. Chemical Sciences, **Giselle Rosquete - Pina**, *Effects of the Molecular Environment on UV-Visible Spectra and the Electronic Structure of Polymethine Systems*, Universidad de La Habana, Facultad de Química, La Habana, Cuba, 2000.
7. Dr. Chemical Sciences, **Annia Galano - Jiménez**, *Modeling of Chemical Systems by Different Quantum Mechanical Methods*, Universidad de La Habana, Facultad de Química, La Habana, Cuba, 2000.

8. Dr. Chemical Sciences, **Anabel Lam - Barandela**, *Theoretical Modeling of Zeolite Materials and Reactions*, Universidad de La Habana, Instituto de Materiales y Reactivos, La Habana, Cuba, 2001.
9. Dr. Chemical Sciences, **Ramón Carrasco - Velar**, *New Atomic and Molecular Descriptors for Activity – Structure Studies. Applications*. Centro de Química Farmacéutica, La Habana, Cuba 2003.
10. Dr. Chemical Sciences, **Edelsys Codorniu - Hernández**, *Theoretical models on condensation and reactivity of flavanol type flavonoids in different molecular environments*, Universidad de La Habana, Facultad de Química, La Habana, Cuba, 2005.
11. Dr. Chemical Sciences, **Yovani Marrero - Ponce**, *Molecular quadratic indexes: applications to molecular design in QSAR studies*, Universidad de La Habana, Facultad de Química, La Habana, Cuba, 2005.
12. Doktor Naturwissenschaften, **Elsa Sánchez - García**, *Computational Study of Weakly Interacting Complexes*, Ruhr-Universität Bochum, Fakultät für Chemie, Bochum, Germany, 2006.
13. Dr. Chemical Sciences, **Miguel Ángel Sirés - Mitjans**, *Effect of core electron polarization on semiempirical calculations of molecular properties*, Universidad de Cádiz, Cádiz, España, 2006.
14. Dr. Chemical Sciences, **Yoanna María Álvarez Ginarte**, *In silico procedure for obtaining QSAR models of anabolic and androgenic steroids*, Universidad de La Habana, Facultad de Química, La Habana, Cuba, 2008.
15. Dr. Chemical Sciences, **Alexis Otero Calvi**, *Modelos teóricos de la estructura molecular y propiedades electrónicas de compuestos para la separación tecnológica de níquel y cobalto con ácidos fosfínicos*, Universidad de La Habana, Facultad de Química, La Habana, Cuba, 2009.
16. Dr. Chemical Sciences, **Rachel Crespo Otero**, *Modelos teóricos de la interacción del óxido nítrico con moléculas de capa cerrada*, Universidad de La Habana, Facultad de Química, La Habana, Cuba, 2009.
17. Dr. Chemical Sciences, **Yoana Pérez Badell**, *Modelación teórica de procesos asociados a la síntesis de zeolitas y oxidación de olefinas dentro de sus cavidades*, Universidad de La Habana, Facultad de Química, La Habana, Cuba, 2010.
18. Dr. Chemical Sciences, **Cercis Morera Boado**, *Modelación teórica de los brasinoesteroides y sus interacciones moleculares*, Universidad de La Habana, Facultad de Química, La Habana, Cuba, 2010.
19. Dr. Chemical Sciences, **Ana Lilian Montero Alejo**, *Nuevas aproximaciones CNDOL para describir las excitaciones electrónicas de nanosistemas*, Universidad de La Habana, Facultad de Química, La Habana, Cuba, 2011.
20. Doctor en Ciencias Médicas, **Erix Wiliam Hernández Rodríguez**, *Modelación Molecular de Rodopsinas Humanas Mutantes asociadas a Retinosis Pigmentaria*, Universidad de Ciencias Médicas de La Habana, Instituto de Ciencias Básicas y Preclínicas “Victoria de Girón”, La Habana, Cuba, 2013.
21. Doctor en Ciencias Químicas, **Germán Miguel Pérez Quintana**, *Desarrollo de metodologías computacionales para el descubrimiento de nuevos receptores peptídicos*, Universidad de La Habana, La Habana, Cuba, 2015.
22. Doctor en Ciencias Químicas, **Ramón Alaín Miranda Quintana**, *Estudios de reactividad química a partir de la teoría del funcional de la densidad conceptual*, Universidad de La Habana, La Habana, Cuba, 2016

**Doctorate students:**

- Marcia Bustamante, Universidad de La Habana, 2002
- Susana González-Santana, Universidad de La Habana, La Habana, 2006
- Marco Martínez González, Universidad de La Habana, La Habana, 2015
- Carlos Manuel de Armas Morejón, Universidad de La Habana, La Habana, 2016
- Gabriela Sánchez Díaz, Universidad de La Habana, La Habana, 2016
- David Hernández Castillo, Universidad de La Habana, 2017
- Roy González Alemán, Universidad de La Habana, 2017

**Labor:**

- Escuela Secundaria Básica "Carlos J. Finlay", Havana, 1963-64, Teacher of Physics.
- Facultad Preparatoria, Universidad de La Habana, Havana, 1965-66, Teacher of General Chemistry
- Facultad de Ciencias, Universidad de La Habana, Havana, 1966-67, non graduate instructor in Inorganic Chemistry
- Facultad de Ciencias, Universidad de La Habana, Havana, 1967-68, non graduate instructor in Physical Chemistry
- Ministry of Education, Havana, 1969-76, Advisor in Science Policy for Higher Education
- Facultad de Ciencias, Universidad de La Habana, Havana, 1969-77, Teacher in Physical Chemistry
- Ministry of Higher Education, Havana, 1976-82, Advisor in Science Policy for Higher Education
- Facultad de Química, Universidad de La Habana, Havana, 1977-83, Associate Professor in Physical Chemistry
- Academia de Ciencias de Cuba, Institute of Chemistry, Havana, 1983-1986, Vice Chairman of Institute, Full Researcher
- Facultad de Química, Universidad de La Habana, Havana, 1983-, Full Professor in Physical Chemistry
- Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts, USA, 2012, 2014, Visiting Scholar
- Department of Chemistry and Chemical Biology, Johns Hopkins University, Baltimore, Maryland, USA, 2016, Visiting Professor

**Cuban National Scientific Duties:**

- Advisor on Research Policy and Postgraduate Education, Ministry of Education, 1969-76
- Secretary of the National Council of Science Policy in Higher Education, 1972-76
- Member of the National Commission for Science Degrees, 1973-75
- Advisor in the Department of Research Policy in the Ministry of Higher Education, 1976-1978.
- Chairman of the Department of Research Policy in the Ministry of Higher Education, 1978-1982.
- Secretary of the Central Commission for Scientific Categories in the Ministry of Higher Education, 1976-82
- Vice Chairman for Research, Institute of Chemistry and Experimental Biology of the Cuban Academy of Sciences, 1983 - 1986.
- Founder Member, 1978, Executive Secretary, 1978 - 1985, and Deputy Chairman of the *Cuban Chemical Society*, 1985-1996.
- Secretary of the Court for Higher Research Categories in Natural Sciences, Cuban Academy of Sciences, 1983-89
- Chairman of the *Laboratory of Computational and Theoretical Chemistry*, Faculty of Chemistry, Universidad de La Habana, 1986-
- Referee in "Revista Cubana de Química" (1986-), and "Revista CNIC de Ciencias Químicas" (1977-)
- Chairman in the Expertise Committee of the National Project in "Computational Models in Chemistry and Biology" (1986-90)
- Chairman of the National Commission of "Mathematical Methods in Chemistry", for designing the new study plans in Chemistry, 1988-2004
- Member of the court for the National Award for Science and Technology Book (1990)
- Member of the Scientific Council of the Faculty of Chemistry, University of Havana, 1990-
- Chairman of the Expertise Committee of the National Project in Natural Sciences "Molecular Design" (1991-1992)

- Member of the *Cuban Physical Society*, 1991-
- Chairman of the court for the National Award for Science and Technology Book (1992)
- Chairman of the Scientific Council of the Faculty of Chemistry, University of Havana, 1995-2004
- Member, 1986 - 1996, and Chairman of the Court for Higher Research Categories in the University of Havana, 1997 - 2005
- Member of the Court for Higher Educational Categories in the Higher Institute for Nuclear Sciences and Technology, 1997
- Member of the National Commission for Basic Sciences, Agency for Science and Technology, Havana, 1998 – 99
- Coordinator for Chemistry in the National Commission for Basic Sciences, Ministry of Science, Technology and Environment, Havana, 2001 - 02
- Member of the National Commission for Bioinformatics, Ministry of Science, Technology and Environment, Havana, 2001 – 02
- Chairman of the *Virtual Center of Bioinformatics*, Universidad de La Habana, Havana, 2001 –
- Member of the Scientific Council of the “Universidad de Ciencias de la Información”, Havana, 2003
- Chairman of the National Commission of "Mathematical and Computer Sciences in Chemistry", for designing the new study plans in Chemistry, 2004-2016
- Member of the Scientific Council of the Universidad de La Habana, Havana, 2004 –
- Member of the permanent court for doctorate degrees of Chemistry, 2004-
- Chairman of the Scientific Council of the Universidad de La Habana, Havana, 2005 –
- Member of the Cuban scientific and educational delegation to Switzerland, Havana, 2006.
- Academician, Academia de Ciencias de Cuba, Havana, 2006.
- Member of the Advising Technical Council of the Ministry of Higher Education, Havana, 2008 -
- Vicepresident, Cuban Chemical Society, Havana, 2009 -2012
- Member of the National Commission for Improving the Academia de Ciencias de Cuba, Havana, 2010
- President of the Cuban Chemical Society, Havana, 2012-2016
- Coordinator of the Section of Natural and Exact Sciences of the Cuban Academy of Sciences, Havana, 2012-
- Coordinator of the Academic Committee of the Collaborative Curricular Doctoral Program on Bioinformatics, Universidad de La Habana, Havana, 2013-2017
- Member of the experts committee of the National Program of Basic Sciences, Universidad de La Habana, Havana, 2013-
- Member of the expert team for the "Propuesta de bases organizativas para la realización de experimentos a favor de la inserción de los resultados de la ciencia e innovación tecnológica en las entidades del MES, en el desarrollo económico y social del país", MES, May, 2013.
- Writer of opinion articles on science, technology, innovation and science policy in Cubadebate, 2015 - (<http://www.cubadebate.cu/autor/luis-a-montero-cabrera/>)

#### **International Scientific Duties:**

- Member of the International Editorial Board of the Journal *Sovremennaya Visshaia Shkola* (Contemporary Higher Education), Warsaw, 1974-78
- Member of the International Expert Group on Science Policy in Higher Education, Berlin, 1976-1982
- Cuban representative in the expertise committee of the international project *Quantum Chemistry* (1986-90).
- Visiting Researcher in the *Sektion Chemie*, Technische Universität Dresden, Dresden, Germany, 1986.
- Representative of the *World Association of Theoretical Organic Chemists* for Central America and the Caribbean Basin, 1988-1993.
- Visiting Professor in the *Institute of Inorganic Chemistry*, University of Milano, Milano, Italy, 1989.
- Referee of the *Journal of Molecular Structure (THEOCHEM)*, 1990-
- Member of the *American Chemical Society*, 1991-1995
- Visiting Researcher in the *Laboratoire de Dynamique des Interactions Moleculaires (CNRS)*, Université Pierre et Marie

- Curie, Paris, France, 1991.
- Visiting Researcher in the *Dep. of Quantum Chemistry*, Uppsala University, Uppsala, Sweden, 1991.
  - Referee of *Folia Chimica Theoretica Latina*, 1992-
  - Visiting Researcher in the *Instituto de Estructura de la Materia*, CSIC, Madrid, Spain, 1992-93.
  - Referee of the *International Journal of Quantum Chemistry*, 1993-
  - Referee of *The Journal of the American Chemical Society*, 1995-
  - Cuban Director of the project *Theoretical Chemistry in Low Cost Computers: Creation and Education* by the Swedish Agency for Research Cooperation with Developing Countries, 1991-1994.
  - Visiting Professor in the Universidad Nacional de Colombia in Bogota, Bogota, Colombia, 1994.
  - Invited member to the jury for a doctorate thesis dissertation of Dr. Antonio González in the Universidad de Las Palmas de Gran Canaria, Dep. of Physics, Spain 1994.
  - Chairman of the UNESCO Chair Project in the Iberoamerican Laboratory of Computational Chemistry and Molecular Design, Havana, Cuba, and Madrid, Spain, 1994
  - Member of the Academy of Sciences of New York, New York, USA, 1994.
  - Visiting Researcher in the *Laboratoire de Dynamique des Interactions Moleculaires (CNRS)*, Université Pierre et Marie Curie, Paris, France, 1994.
  - Visiting Professor in the *Institut für Organische Chemie*, Technische Universität Dresden, Dresden, Germany, 1995.
  - Invited member to the jury for a doctorate thesis dissertation of Dr. Flor M. Poveda, in the Universidad Nacional de Colombia, Bogota, Dep. of Chemistry, Colombia, 1995.
  - Visiting Researcher in the *Instituto de Estructura de la Materia*, CSIC, Madrid, Spain, 1995.
  - Visiting Professor in the Dep. of Applied Physical Chemistry, Universidad Autónoma de Madrid, Madrid, Spain, 1995.
  - Visiting Professor in the Department of Chemistry, Cornell University, Ithaca, NY, USA, 1996.
  - Visiting Researcher in the Center for Theoretical Studies of Physical Systems, Clark Atlanta University, Atlanta, GA, USA, 1996 -.
  - Visiting Researcher in the *Grupo de Modelización y Diseño Molecular*, Universidad de Granada, Granada, Spain, 1996.
  - Visiting Researcher in the *The Royal Institution of Great Britain*, London, UK, 1996.
  - Referee of the *Journal of Physical Chemistry*, 1995-
  - Visiting Professor in the *Lehrstuhl Theoretische Chemie*, Friedrich-Alexander Universität, Erlangen - Nürnberg, Germany, 1997.
  - Visiting Researcher in the *Dep. of Physical Chemistry*, Universidad de Santiago de Compostela, Santiago de Compostela, Spain, 1997.
  - Visiting Professor in the Universidad Nacional de Colombia in Medellín, Medellín, Colombia, 1997.
  - Visiting Professor in the Department of Chemistry, University of Arkansas, Fayetteville, AR, USA, 1998.
  - Visiting Professor in the Department of Chemistry, Cornell University, Ithaca, NY, USA, 1998.
  - Associate Researcher in the Center for Theoretical Studies of Physical Systems, Clark Atlanta University, Atlanta, GA, USA, 1998 -.
  - Visiting Researcher in the Facultad de Ciencias de la Computación, Benemérita Universidad Autónoma de Puebla, Puebla, México, 1998.
  - Member of the editorial board of *Folia Chimica Theoretica Latina*, Madrid, Spain, 1998-2003
  - Visiting Professor in the *Institut für Organische Chemie*, Technische Universität Dresden, Dresden, Germany, 1999.
  - Visiting Researcher in the *Max Planck Institut für Strahlenchemie*, Mülheim, Germany, 1999.
  - Invited Professor in the *Institut für Organische Chemie*, Ruhr Universität, Bochum, Germany, 1999.
  - Invited Professor in the *Institut für Anorganische Chemie*, Universität Münster, Münster, Germany, 1999.
  - Invited Professor in the *Institut für Organische Chemie*, Universität Bremen, Bremen, Germany, 1999.
  - Visiting Professor in the *Lehrstuhl Theoretische Chemie*, Friedrich-Alexander Universität, Erlangen - Nürnberg, Germany, 1999.
  - Visiting Researcher in the *Grupo de Modelización y Diseño Molecular*, Universidad de Granada, Granada, Spain, 1999
  - Visiting Professor in the Universidad Nacional Mayor de San Andrés, La Paz, Bolivia, 1999.
  - Visiting Professor in the Facultad de Ciencias, Universidad Industrial de Santander, Bucaramanga, Colombia, 2000
  - Visiting professor in the Lehrstuhl für Organische Chemie 2, Ruhr-Universität Bochum, Bochum, Germany, 2000

- Invited Professor in the *Institut für Anorganische Chemie*, Universität Münster, Münster, Germany, 2000.
- Invited Professor in the *Institut für Organische Chemie*, Universität Bremen, Bremen, Germany, 2000.
- Visiting researcher in the Davy – Faraday Laboratory, *The Royal Institution of Great Britain*, London, UK, 2000.
- Invited professor in the Dep. of Chemistry, University of York, York, UK, 2000.
- Invited member to the jury for a doctorate thesis dissertation of Dr. Edgar Daza, in the Universidad Nacional de Colombia, Bogota, Dep. of Chemistry, Colombia, 2000.
- Visiting professor, Facultad de Ingeniería, Universidad Nacional de Colombia, Manizales, Colombia, 2001
- Coordinator of the “Seminar on Modelling of Molecules and Biomolecules: State of the Art and Perspectives”, Fundación Ramón Areces, Madrid, 2001.
- Coordinator of the Project Liebig – Reynoso for improving chemical education in Cuba, Havana, 2001.
- Visiting professor in the *Institut für Organische Chemie*, Universität Bremen, Bremen, Germany, 2002.
- Invited delegation on bioinformatics by the BMBF (Federal Ministry for Education and Research), Federal Republic of Germany, Germany, 2002.
- Invited member to the jury for a doctorate thesis dissertation of Dr. Martha Daza, in the Universidad Nacional de Colombia, Bogota, Dep. of Chemistry, Colombia, 2002.
- Visiting researcher in the Davy – Faraday Laboratory, *The Royal Institution of Great Britain*, London, UK, 2003.
- Visiting professor in the *Institut für Organische Chemie*, Universität Bremen, Bremen, Germany, 2003.
- Visiting professor in the *Instituto de Química Computacional*, Universidad de Girona, Girona, Spain, 2003.
- Visiting professor in the *Departamento de Química Física Aplicada*, Universidad Autónoma de Madrid, Madrid, Spain, 2003.
- Invited professor in the *Facultad de Química*, Universidad de Cadiz, Cadiz, Spain, 2003.
- Invited professor in the *Estación Experimental del Zaidín*, Consejo Superior de Investigaciones Científicas, Granada, Spain, 2003.
- Invited professor in the *Instituto de Estructura de la Materia*, Consejo Superior de Investigaciones Científicas, Madrid, Spain, 2003.
- Invited professor in the Wolfson Institute of the University College of London, London, UK, 2003.
- Invited professor in the Faculty of Sciences, Université Henri Poincaré, Nancy, France, 2003.
- Visiting professor in the *Institut für Organische Chemie*, Universität Bremen, Bremen, Germany, 2004.
- Visiting professor in the *Department of Chemistry*, University of Oxford, Oxford, UK, 2004.
- Visiting Professor in the Universidad Nacional de Colombia in Bogota, Bogota, Colombia, 2004.
- Visiting Professor in the Dep. of Applied Physical Chemistry, Universidad Autónoma de Madrid, Madrid, Spain, 2005.
- Visiting Professor in the Facultad de Química, Universidad Autónoma de Chihuahua, Chihuahua, México, 2005.
- Visiting professor in the *Institut für Organische Chemie*, Universität Bremen, Bremen, Germany, Feb. 2006.
- Visiting researcher in the Davy – Faraday Laboratory, *The Royal Institution of Great Britain*, London, UK, 2006.
- Visiting Professor in the Dep. of Applied Physical Chemistry, Universidad Autónoma de Madrid, Madrid, Spain, 2006.
- Visiting Professor in the Universidad Autónoma de Ciudad Juárez, Ciudad Juárez, México, 2006.
- Visiting Professor in the Facultad de Química, Universidad Autónoma de Chihuahua, Chihuahua, México, 2006.
- Invited member to the jury for a doctorate thesis dissertation of Dr. Elsa Sánchez García, in the Ruhr-Universität Bochum, Fakultät für Chemie, Bochum, Germany, 2006.
- Visiting professor in the *Institut für Organische Chemie*, Universität Bremen, Bremen, Germany, Sept., 2006.
- Visiting professor in the *Laboratory of Ultrafast Spectroscopy, Institute of Chemical Sciences and Engineering (ISIC), EPFL*, Lausanne, Switzerland, March, 2007.
- Visiting professor in the Lehrstuhl für Organische Chemie 2, Ruhr-Universität Bochum, Bochum, Alemania, April, 2007
- Visiting professor in the *Institut für Organische Chemie*, Universität Bremen, Bremen, Alemania, April, 2007.
- Visiting professor in the Dep. de Química Física Aplicada, Universidad Autónoma de Madrid, Madrid, España, May, 2007.
- Member of the editorial board of *Journal of Cuban Studies*, London, UK, 2007-
- Visiting professor in the Dep. de Química Física Aplicada, Universidad Autónoma de Madrid, Madrid, España, March - June, 2008.
- Visiting Professor in the Universidad Nacional de Colombia in Bogota, Medellín, Colombia, 2008.



- Visiting professor in the Lehrstuhl für Organische Chemie 2, Ruhr-Universität Bochum, Bochum, Alemania, April, 2009
- Visiting professor in the Dep. de Química Física Aplicada, Universidad Autónoma de Madrid, Madrid, España, May, 2009.
- Visiting professor, Departamento de Física, Universidad de Chile, Santiago, March - April, 2010
- Visiting professor in the Lehrstuhl für Organische Chemie 2, Ruhr-Universität Bochum, Bochum, Alemania, April, 2010
- Visiting professor in the Dep. de Química Física Aplicada, Universidad Autónoma de Madrid, Madrid, España, May, 2010.
- Visiting professor in the Institut für Chemische Technologien und Analytik, Technische Universität Wien, Viena, Austria, February, 2011.
- Visiting professor in the *Laboratory of Computational Chemistry and Biochemistry, Institute of Chemical Sciences and Engineering (ISIC), EPFL*, Lausanne, Suiza, February, 2011.
- Visiting professor in the Dep. de Química Física Aplicada, Universidad Autónoma de Madrid, Madrid, España, March, 2011.
- Visiting professor in the University of Venda, Thohoyandou, Republic of Southafrica, September, 2011
- Visiting professor in the Dep. de Química Física Aplicada, Universidad Autónoma de Madrid, Madrid, España, May, 2012.
- Visiting professor in the *College of Chemistry and Molecular Engineering, Peking University*, June 2012.
- Visiting professor in the Institut für Chemische Technologien und Analytik, Technische Universität Wien, Viena, Austria, June, 2012.
- Santander Visiting Scholar in the David Rockefeller Center for Latin American Studies, Harvard University, Cambridge, Massachusetts, USA, 2012.
- Visiting professor in the Dep. de Química Física Aplicada, Universidad Autónoma de Madrid, Madrid, España, March, 2013.
- Invited Professor, Dep. of Chemistry of the University College of London, London, UK, 2013
- Invited Professor, Dep. of Biology, Fluminense Federal University, Niteroi, Brasil, 2013
- Visiting professor, Dep. of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts, USA, 2014
- Invited professor, Donostia International Physics Center, Donostia, Basque Country, Spain, 2014
- Invited professor, Departamento de Bioinformática, Universidad de Talca, Talca, Chile, 2015.
- Invited Professor, Department of Chemistry, University of Coimbra, Coimbra, Portugal, 2015
- Member of the Royal Society of Chemistry, London, UK, 2016-
- National Representative of the IUPAC Physical and Biophysical Division, IUPAC, 2016-2017
- Visiting Professor, Department of Chemistry, Johns Hopkins University, Baltimore, USA, 2016.
- Member of the American Association for the Advancement of Science (AAAS), Washington, DC, 2017 –
- Invited professor, Donostia International Physics Center, Donostia, Basque Country, Spain, 2017
- Invited professor, Donostia International Physics Center, Donostia, Basque Country, Spain, 2018
- Invited professor, Departamento de Bioinformática, Universidad de Talca, Talca, Chile, 2018.

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173. Miranda-Quintana, R. A.; González, M. M.; Hernández-Castillo, D.; Montero-Cabrera, L. A.; Ayers, P. W.; Morell, C., Conceptual DFT analysis of the regioselectivity of 1,3-dipolar cycloadditions: nitrones as a case of study. Journal of Molecular Modeling **2017**, 23 (8), 236.

### Scientific Meetings:

The most important are in *italics*.

1. Conferencia de Química, Santiago de Cuba, 1967\*
2. Seminario Preparatorio del Congreso Cultural de La Habana, La Habana, 1967
3. Seminario Científico del Centro Nacional de Investigaciones Científicas, La Habana, 1969\*
4. Conferencia de Química, Santiago de Cuba, 1969\*
5. Seminario Interdisciplinario de Educación Permanente, La Habana, 1970
6. Congreso Nacional de Educación, La Habana, 1971
7. 6th. International Symposium on Cellulose Chemistry and Technology, Iasi, Rumanía, 1971
8. Seminario Científico del Centro Nacional de Investigaciones Científicas, La Habana, 1971\*
9. Forum Científico Nacional de Estudiantes Universitarios, La Habana, 1971\*\*
10. Conferencia de Química, Santiago de Cuba, 1972\*
11. Expert Meeting on Organization of Educación, Ulan Bator, Mongolia, 1973\*
12. Seminario Científico del Centro Nacional de Investigaciones Científicas, La Habana, 1973\*
13. International Expert Meeting on Combination of Learning and Labor in Educación, La Habana, 1974\*\*
14. 3rd. Meeting of the Editorial Council of the journal *Sovremennaya Visshaia Shkola* (La Educación Superior Contemporánea), Sofia, Bulgaria, 1974\*
15. Conferencia de Química, Santiago de Cuba, 1974
16. 2nd. International Symposium on the Chemistry of Non Benzenoid Aromatic Compounds, Lindau-Bodensee, Germany, 1974\*
17. 4th. Meeting of the Editorial Council of the journal *Sovremennaya Visshaia Shkola* (La Educación Superior Contemporánea), Sosopol, Bulgaria, 1974\*
18. 9th. Conference of Ministries of Higher Education, La Habana, 1974\*\*
19. Forum Científico Nacional de Estudiantes Universitarios, Santa Clara, 1974
20. 5th. Meeting of the Editorial Council of the journal *Sovremennaya Visshaia Shkola* (La Educación Superior Contemporánea), Budapest, Hungría, 1975\*
21. 6th. Meeting of the Editorial Council of the journal *Sovremennaya Visshaia Shkola* (La Educación Superior Contemporánea), Siofok, Hungría, 1975\*
22. Seminario Científico del Centro Nacional de Investigaciones Científicas, La Habana, 1975\*
23. 7th. Meeting of the Editorial Council of the journal *Sovremennaya Visshaia Shkola* (La Educación Superior Contemporánea), Egsdorf (Berlin), Germany, 1976\*
24. 1st. Meeting of the International Expert Group on Science Policy in Higher Education, Magdeburg, Germany, 1976\*
25. 8th. Meeting of the Editorial Council of the journal *Sovremennaya Visshaia Shkola* (La Educación Superior Contemporánea), Potsdam, Germany, 1976\*
26. Conferencia de Química, Santiago de Cuba, 1977\*

27. 9th. Meeting of the Editorial Council of the journal *Sovremennaya Visshaia Shkola* (La Educación Superior Contemporánea), La Habana, 1977\*\*
28. 3rd. Meeting of the International Expert Group on Science Policy in Higher Education, Cotbus, Germany, 1977\*
29. Seminario Científico del Centro Nacional de Investigaciones Científicas, La Habana, 1977\*
30. 4th. Meeting of the International Expert Group on Science Policy in Higher Education, Vespem, Hungría, 1978\*
31. *Asamblea Constitutiva de la Sociedad Cubana de Química, La Habana, 1978\*\**
32. 5th. Meeting of the International Expert Group on Science Policy in Higher Education, Prague, Checoslovaquia, 1979\*
33. Taller de Investigaciones Científicas sobre la Educación Superior, Camagüey, 1979\*\*
34. 6th. Meeting of the International Expert Group on Science Policy in Higher Education, Varna, Bulgaria, 1979\*
35. Seminario Nacional de la Educación Superior, La Habana, 1979
36. 7th. Meeting of the International Expert Group on Science Policy in Higher Education, Halle, Germany, 1980\*
37. International Döbereiner Symposium, Jena, Germany, 1980
38. Semana Científica del Instituto de Química y Biología Experimental, Academia de Ciencias de Cuba, La Habana, 1980\*
39. Seminario Científico del Centro Nacional de Investigaciones Científicas, La Habana, 1980\*
40. *28th. Congress of the International Union of Pure and Applied Chemistry, Vancouver, Canada, 1981\**
41. Simposio del Furfural, La Habana, 1981\* #
42. Conferencia Científica de la Universidad de La Habana, La Habana, 1981\* #
43. Conferencia de Investigaciones Científicas acerca de la Educación Superior, Camagüey, 1981\*\*
44. Seminario Nacional de la Educación Superior, La Habana, 1981\*
45. 9th. Meeting of the International Expert Group on Science Policy in Higher Education, Budapest, Hungría, 1982\*
46. *Congreso Nacional de la Sociedad Cubana de Química, La Habana, 1982\*\**
47. Conferencia de Química, Santiago de Cuba, 1982
48. Escuela Latinoamericana de Química Teórica, Mexico D.F., Mexico, 1983
49. Foro Científico Nacional de la Academia de Ciencias de Cuba, La Habana, 1983\*
50. Coloquio sobre el Impacto de la Técnicas de Cómputo Electrónico en la Investigación Química y Biológica, La Habana, 1983\*\* #
51. Conferencia de Ciencias Sociales y Naturales de la Universidad Central de Las Villas, Santa Clara, 1984\*
52. Simposio sobre Análisis Estructural Orgánico mediante Técnicas Espectroscópicas, La Habana, 1984\*
53. Escuela Latinoamericana de Química Teórica, Caracas, Venezuela, 1984\* #
54. *Conferencia de Química y II Congreso de la Sociedad Cubana de Química, Santiago de Cuba, 1985\*\* #*
55. *5th. International Congress on Quantum Chemistry, Montreal, Canada, 1985\**
56. Semana Científica del Instituto de Química de la Academia de Ciencias de Cuba, La Habana, 1985\*
57. Escuela Cubana de Química Teórica, Santa Clara, 1986\*\* #
58. International Meeting on Quantum Chemistry, Novosibirsk, Rusia, 1986\* #
59. Seminario Cubano sobre Biotecnología, La Habana, 1986\*
60. Conferencia Científica de Ciencias Naturales de la Universidad de La Habana, La Habana, 1986\*
61. V Escuela Latinoamericana de Química Teórica, La Habana, Cuba, 1986\*\* #
62. Escuela Cubana de Química Teórica, Santiago de Cuba, 1987\*\* #
63. Congreso de Ciencias Farmacéuticas, La Habana, 1987\* #
64. *Congress of the World Association of Theoretical Organic Chemists, Budapest, Hungría, 1987\**
65. 2nd. Symposium on Chemical Reactivity and Elementary Processes, Liblice, Checoslovaquia, 1987\*

66. Taller Internacional sobre Enseñanza de la Química, La Habana, 1988<sup>\*\* #</sup>
67. Escuela Cubana de Química Teórica, Pinar del Río, 1988<sup>\*\*#</sup>
68. International Meeting on Quantum Chemistry, Burgas, Bulgaria, 1988<sup>\* #</sup>
69. International Symposium on Quantum Chemistry, Tratraska Lomnica, Checoslovaquia, 1988<sup>\*</sup>
70. 5th. International Symposium on Furan Chemistry, Riga, Letonia, 1988<sup>\*</sup>
71. Congreso de Informática'88, La Habana, 1988<sup>\*</sup>
72. Seminario Científico del Centro Nacional de Investigaciones Científicas, La Habana, 1988<sup>\*</sup>
73. Taller Nacional de Aplicaciones de la Computación a la Biología, La Habana, 1988<sup>\*\*</sup>
74. Reunión Científica de Profesores del Instituto Superior Pedagógico de Pinar del Río, Pinar del Río, 1988<sup>\* #</sup>
75. Symposium on the Theory of Environmental Effects on Molecular Structure and Chemical Reactivity, St. John's, Canada, 1989<sup>\* #</sup>
76. Escuela Cubana de Química Teórica, Camagüey, 1989<sup>\*\* #</sup>
77. Coloquio de Computación y Matemática Aplicada a las Ciencias Naturales, La Habana, 1989<sup>\*</sup>
78. Workshop on Aspects of Molecular Graphics, Pisa, Italia, 1989<sup>\* #</sup>
79. Taller Internacional sobre Enseñanza de la Química, La Habana, 1990<sup>\*\* #</sup>
80. Conferencia de Química, Santiago de Cuba, 1990<sup>\* #</sup>
81. Jornada Científica del Instituto Superior Pedagógico de Pinar del Río, Pinar del Río, 1990<sup>\* #</sup>
82. Seminario 25 Aniversario del Instituto Cubano de Investigaciones de Derivados de la Caña de Azúcar, La Habana, 1990
83. Jornada de Aplicaciones de la Computación en Química, Santiago de Cuba, 1990<sup>\* #</sup>
84. Jornada Científica Estudiantil de la Facultad de Química y de la Universidad de La Habana, La Habana, 1990<sup>\*</sup>
85. International Symposium on Applied Theoretical Chemistry, La Habana, 1990<sup>\*\*</sup>
86. *2nd. Congress of the World Association of Theoretical Organic Chemists, Toronto, Canada, 1990\*#*
87. *29<sup>no</sup>. Congreso de Químicos Teóricos de Expresión Latina, Roma, Italia, 1990\**
88. Scientific Meeting of Graduates from USSR Higher Education Centers (invited scientist and chairman of a session), La Habana, 1990<sup>\*</sup>
89. 7th. International Congress of Quantum Chemistry, Menton, Francia, 1991<sup>\*</sup>
90. 14th. Austin Symposium on Molecular Structure, Austin, Texas, USA, 1991 #
91. International School of Theoretical Chemistry in Pinar del Río, Pinar del Río, Cuba, 1992<sup>\*\* #</sup>
92. Sanibel Symposium, St. Augustin, Florida, USA, 1993<sup>\*</sup>
93. Congress of the International Society of Theoretical Chemical Physics, Girona, España, 1993<sup>\*\*#</sup>
94. Congreso de la Sociedad Cubana de Física, La Habana, Cuba, 1994<sup>\*</sup>
95. Conferencia de Química, Santiago de Cuba, Cuba, 1994<sup>\*#</sup>
96. Congreso de Química del Sureste de México, Mérida, México, 1995<sup>\*</sup>
97. Symposium on Experimental and Computational Chemistry: The Fruitful Interplay, Erlangen, Germany, 1995.
98. Escuela Iberoamericana de Química Computacional y Diseño Molecular, La Habana, Cuba, 1996<sup>\*\*</sup>
99. Sanibel Symposium, St. Augustin, Florida, USA, 1996.<sup>\*</sup>
100. 16th. Austin Symposium on Molecular Structure, Austin, Texas, USA, 1996 #
101. La Cristalografía y la Industria Farmacéutica, Granada, España, 1996#.
102. Conferencia de Química, I Simposio de Química Computacional y Diseño Molecular, Santiago de Cuba, 1996<sup>\*\*</sup>.
103. Annual Meeting of the Polar Solids Discussion Group, The Royal Society of Chemistry, University of Sussex, Brighton, UK, 1996.
104. Computer Modelling of Inorganic Chemicals: One Day Meeting, The Royal Society of Chemistry, Londres, 1996.
105. Symposium on the 100th Anniversary of the Discovery of the Electron, Instituto de Materiales y Reactivos, Universidad de La Habana, La Habana, 1997#
106. International School on Computational Modeling of Molecules, Instituto Superior de Ciencias y Tecnología Nuclear,

- La Habana, 1997#
107. 5<sup>th</sup> Chemical Congress of North America, Cancún, México, 1997#
  108. 2<sup>da</sup> Escuela Iberoamericana de Química Computacional y Diseño Molecular, La Habana, Cuba, 1998\*\*.
  109. 3<sup>rd</sup>. European Workshop on Quantum Systems in Physics and Chemistry, Granada, España, 1998#
  110. XI Congreso de la Asociación Química de Colombia, Bucaramanga, Colombia, 1998#.
  111. XXIV Congreso Internacional de Químicos Teóricos de Expresión Latina, Puebla, México, 1998#.
  112. Fotociencias'99, La Habana, Cuba, 1999\*\*#.
  113. II Taller Iberoamericano sobre Educación en Ciencia de Materiales, La Habana, Cuba, 1999#
  114. Humboldt Symposium on Chemistry, La Habana, Cuba, 1999\*\*#
  115. 4<sup>th</sup>. European Workshop on Quantum Systems in Physics and Chemistry, Marly-le-Roi, France, 1999#
  116. 4<sup>th</sup> South European Conference on Atomic and Molecular Physics, Gandia, España, 1999#
  117. "Alexander von Humboldt: un enfoque universal de las ciencias", Caracas, Venezuela, 1999#
  118. III Simposio Internacional de Estrés Oxidativo, La Habana, Cuba, 1999#
  119. Photodynamics from Isolated Molecules to Condensed Phases, Havana, Cuba, 2000#
  120. 3eros. Seminarios de Estudios Avanzados en Diseño Molecular, La Habana, Cuba, 2000\*\*#.
  121. V Taller Iberoamericano de Catálisis Computacional, La Habana, Cuba, 2000#
  122. 3er. Congreso Nacional de Alimentación y Nutrición, La Habana, Cuba, 2001#.
  123. I Taller Nacional de Bioinformática, La Habana, Cuba, 2001#\*\*
  124. IV Congreso Internacional de Química de la Sociedad Cubana de Química, Symposium on Macromolecular Chemistry, La Habana, 2001#
  125. 12<sup>th</sup> Interamerican Photochemical Conference, Ascochinga (Córdoba), Argentina, 2001#
  126. Seminario Taller sobre Gestión de la Cooperación Internacional Universitaria, Centro de Estudios de la Educación Superior, Universidad de La Habana, La Habana, Cuba, 2001\*
  127. Escuela Internacional de Nanoestructuras, Instituto de Materiales y Reactivos, Universidad de La Habana, La Habana, Cuba, 2001#
  128. Seminario acerca de la Modelización de Moléculas y Biomoléculas: Estado Actual y Perspectivas, Fundación Ramón Areces, Madrid, 2001, \*\*,#
  129. Fotociencias 2002, La Habana, Cuba, 2002\*\*.
  130. IV Seminarios de Estudios Avanzados en Diseño Molecular y Bioinformática, La Habana, Cuba, 2002\*\*#.
  131. 2nd. International Symposium on Photodynamics, Havana, Cuba, 2002#
  132. International Congress "Informática 2002", Havana, Cuba, 2002#.
  133. IX Escuela Internacional de Ciencia y Tecnología de Materiales, La Habana, Cuba, 2002#
  134. Seminario sobre Bioinformática en el Sistema de Salud Pública de Cuba, La Habana, Cuba, 2002#,\*\*
  135. Seminario Científico por el XL Aniversario del Instituto de Ciencias Básicas y Preclínicas "Victoria de Girón", La Habana, Cuba, 2002#
  136. Symposium on Systems Biology, La Habana, Cuba, 2002#
  137. Simposio Cuba – UK de Bioinformática, La Habana, Cuba, 2002\*\*#
  138. Simposio Cuba – Francia de Bioinformática, La Habana, Cuba, 2003\*\*#
  139. Frontiers in Chemical Biology: Biomolecular Dynamics and Force Generation, University of Manchester, Manchester, UK, 2003\*.
  140. V Simposio de Estrés Oxidativo, Instituto Superior de Ciencias Médicas de La Habana, La Habana, Cuba, 2003#.
  141. V Seminarios de Estudios Avanzados en Diseño Molecular y Bioinformática, La Habana, Cuba, 2004\*\*.
  142. 3rd. International Meeting on Photodynamics, Havana, Cuba, 2004\*
  143. 5<sup>th</sup>. International Congress on Chemistry and Chemical Engineering, Havana, Cuba, 2004#.
  144. Coloquio sobre Biología de Sistemas en Cuba: retos y oportunidades, La Habana, Cuba, 2004\*\*,#
  145. Seminario Nacional de Bioinformática, La Habana, Cuba, 2005\*\*#
  146. XXXI Congreso de Químicos Teóricos de Expresión Latina, Isla Margarita, Venezuela, 2005#
  147. Simposio Internacional "Conocimiento, ciencia y educación superior", La Habana, Cuba, 2005#
  148. Cuba – UK Symposium on Chemistry and Life Sciences, La Habana, 2006\*\*#
  149. VI Seminarios de Estudios Avanzados en Diseño Molecular y Bioinformática, La Habana, Cuba, 2006\*\*.

150. XXXII Congreso Internacional de Químicos Teóricos de Expresión Latina, Costas de Cartago, Túnez, 2006\*\*
151. Seminario de Ciencias Criminalísticas, Havana, 2006#
152. Seminario Cuba – Malasia de Bioinformática, Havana, 2006#
153. V Jornada por la Cultura Científica dedicada a las Ciencias Exactas y al periodismo científico, Havana, 2007#
154. II Congreso Nacional de Bioinformática, Havana, 2007\*\*
155. XXXIII Congreso Internacional de Químicos Teóricos de Expresión Latina, Havana, Cuba, 2007\*\*
156. Simposio Cuba – Flandes de Bioinformática, Santa Clara, Cuba, 2008#
157. Universidad 2008, Havana, 2008#
158. XXXIV Congreso Internacional de Químicos Teóricos de Expresión Latina, Calabria, Italia, 2008#
159. VII Seminarios de Estudios Avanzados en Diseño Molecular y Bioinformática, La Habana y Varadero, Cuba, 2009\*\*
160. Nanociencias 2009, La Habana, Cuba, 2009#\*\*
161. Photodynamics 2010, La Habana, Cuba#
162. Frontiers in Chemistry, Paris, 2010, France
163. TECH CONNECT WORLD 2010, Anaheim, California, 2010, USA#
164. 3er Seminario Internacional de Nanociencias y Nanotecnologías, La Habana, Cuba, 2010#
165. XXXVI Congreso Internacional de Químicos Teóricos de Expresión Latina, Anglet, France, 2010#
166. Science - Bridge Between Austria and Cuba, La Habana, Cuba, 2010#
167. Seminar of DFG Forschergruppe on Molecular Interactions, Bochum, Germany, 2011
168. VIII Seminarios de Estudios Avanzados en Diseño Molecular y Bioinformática, La Habana y Varadero, Cuba, 2011\*\*#
169. XX Conferencia Internacional de Química, Santiago de Cuba, Cuba, 2011#
170. 2nd Peking University Forum on the Frontiers of Nanochemistry, Beijing, China, 2012#.
171. Workshop on Atomic and Molecular Physics, Varadero, Cuba, 2012#.
172. Foro de Innovación Hispano-Alemán de la Idea al Mercado, DAAD, March, 2013, Madrid, España
173. IX Seminarios de Estudios Avanzados en Diseño Molecular y Bioinformática, La Habana y Varadero, Cuba, 2013\*\*#
174. 44<sup>th</sup> World Chemistry Congress, IUPAC, August 2013, Istanbul, Turkey.#
175. 47<sup>th</sup> General Assembly of IUPAC, August 2013, Istanbul, Turkey.\*
176. “The Chemistry of Initiatives: Entrepreneurship in Scientific Institutions”, diciembre de 2013, La Habana, Cuba.\*\*
177. Simposio de la Sociedad Cubana de Física, Havana, 2014#
178. XXI Conferencia Internacional de Química, Santiago de Cuba, Cuba, 2014#
179. Optics-Photonics-Photosciences, Havana, Cuba, 2014#
180. Ciencia y Desarrollo – FLACSO, Universidad de La Habana, Havana, 2014#
181. 21st Conference on Chemistry, Universidad de Oriente, Santiago de Cuba, 2014#
182. Encuentro Internacional por 20 Años de creación de la Casa de Altos Estudios Don Fernando Ortiz: Presente y futuro de las ciencias sociales en Cuba. La Habana, Cuba, 2015#.
183. X Seminarios de Estudios Avanzados en Diseño Molecular y Bioinformática, La Habana y Varadero, Cuba, 2015\*\*#
184. 250th Reunión de la American Chemical Society, Boston, MA, USA, 2015\*#
185. 13th Globelics International Conference, Havana, Cuba, 2015.
186. 9<sup>th</sup> Congress of Science, Technology and Innovation in Chemistry (QUIMICUBA 2015), Havana, Cuba, 2015\*\*
187. 32 Congreso Latinoamericano de Química, Concepción, Chile, 2016#
188. InformEx 2016, New Orleans, LA, USA, 2016#
189. Expociencia 2016, Holguín, Cuba#
190. VI Simposio Internacional de Química, Cayo Santa María, Villa Clara, Cuba, 2016#
191. 252<sup>th</sup> Meeting of the American Chemical Society, Boston, MA, USA, 2016#
192. Off Year 2016 Meeting of Physical and Biophysical Chemistry Division of IUPAC, East Lansing, Michigan, USA, 2016
193. “Sustainable Community Development and STEAM Fields: What We Can Learn from a Changing Cuba”, Rutgers University, Camden, NJ, USA, 2016#
194. Hot Topics in Chemistry, Havana, Cuba, 2017\*\*
195. EMN Summer Meeting, Havana, Cuba, 2017, \*\*,#
196. UNIVERSIDAD 2018, Evento Preparatorio Provincial, La Habana, Cuba, 2017#
197. XI Seminarios de Estudios Avanzados en Diseño Molecular y Bioinformática, La Habana y Varadero, Cuba, 2017\*\*
198. SIGESTIC 2017, Varadero, Cuba, 2017#
199. Hot Topics in Science, Havana, Cuba, 2018\*\*

200. WORKSHOP ON HISTORY OF CHEMISTRY "Dr. LUIS FELIPE LE ROY", Havana, 2018#
201. Taller de Nanociencias, Havana, 2018#
202. 255th ACS National Meeting, New Orleans, USA, 2018# (video conference)
203. 33<sup>rd</sup>. Latin American Congress of Chemistry, Havana, 2018\*\*

\* active participation or submitted paper

\*\* organizer of the meeting

# invited lecturer

***Invited Lectures:***

1. Universidad Nacional Autónoma de Nicaragua, Managua, Nicaragua, 1982
2. Universidad Nacional Autónoma de Nicaragua, León, Nicaragua, 1982
3. Universidad Centroamericana, Managua, Nicaragua, 1982
4. Institute of Polymer Chemistry, Academy of Sciences of Germany, Teltow, Germany, 1983
5. Dresden Technical University, Section of Chemistry, Dresden, Germany, 1983
6. Universidad Nacional Autónoma de México, Facultad de Química, División de Estudios de Postgrado, Mexico D.F., 1983
7. University of Alberta, Dep. of Chemistry, Edmonton, Canada, 1985
8. Dresden Technical University, Section of Chemistry, Dresden, Germany, 1986
9. Joint Institute of Nuclear Research, Dubna, USSR, 1986
10. Central Institute of Chemical Research, Hungarian Academy of Sciences, Budapest, Hungary, 1987
11. Institute of Organic Chemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria, 1987
12. Consejo Superior de Investigaciones Científicas, Instituto de Estructura de la Materia, Madrid, España, 1987
13. Instituto Cubano de Investigaciones de los Derivados de la Caña de Azúcar, La Habana, 1987
14. Instituto de Investigaciones Fundamentales de la Agricultura Tropical, Santiago de las Vegas, Cuba, 1987
15. Consejo Superior de Investigaciones Científicas, Instituto de Estructura de la Materia, Madrid, España, 1988
16. Universidad de Oriente, Facultad de Física, Santiago de Cuba, 1988
17. Centre National de la Recherche Scientifique, Lab. on Dynamics of Molecular Interactions, Université Pierre et Marie Curie, Paris, France, 1988
18. Universidad Complutense de Madrid, Facultad de Química, 1988
19. State University of Moscow, Faculty of Chemistry, Moscow, USSR, 1989
20. Institute of Organic Synthesis of the Latvian Academy of Sciences, Riga, USSR, 1989
21. University of Milan, Institute of Structural Inorganic Chemistry, Milan, Italy, 1989
22. University of Hannover, Institute of Theoretical Chemistry, Hannover, Germany, 1991
23. Dresden Technical University, Institute of Organic and Color Chemistry, Dresden, Germany, 1991
24. Consejo Superior de Investigaciones Científicas, Instituto de Estructura de la Materia, Madrid, España, 1991
25. University of Linköping, Dep. of Physics, Linköping, Sweden, 1991.
26. Centre National de la Recherche Scientifique, Lab. on Dynamics of Molecular Interactions, Université Pierre et Marie Curie, Paris, France, 1991.
27. Instituto Superior de Ciencias y Tecnología Nuclear, Dep. de Física, La Habana, 1992.
28. Facultad de Química, División de Estudios de Postgrado, Universidad Nacional Autónoma de México, México, DF, 1992.
29. Instituto de Física, Benemérita Universidad Autónoma de Puebla, Puebla, México, 1992.
30. Dep. of Chemistry, Baker Laboratory, Cornell University, Ithaca, New York, USA, 1992.
31. Ciclo de Conferencias en Física Atómica y Molecular, Consejo Superior de Investigaciones Científicas, Madrid, España, 1992.
32. Instituto de Química Computacional, Universidad de Gerona, Gerona, España, 1993.
33. Institute of Quantum Chemistry, Uppsala University, Uppsala, Sweden, 1993.
34. Departamento de Química, Universidad de Granada, Granada, España, 1994.
35. Facultad de Ciencias, Universidad Nacional de Colombia, Santa Fe de Bogotá, Colombia, 1994.

36. Departamento de Química, Universidad Nacional de Colombia, Medellín, Colombia, 1994.
37. Departamento de Física, Universidad de Las Palmas de Gran Canaria, Las Palmas, España, 1994.
38. Institut für Organische Chemie, Technische Universität Dresden, Dresden, Germany, 1995.
39. Institut für Physikalische und Theoretische Chemie, Friedrich - Alexander - Universität Erlangen-Nürnberg, Erlangen, Germany, 1995.
40. Facultad de Ciencias, Universidad Nacional de Colombia, Santafe de Bogota, Colombia, 1995.
41. Facultad de Ingeniería, Universidad Industrial de Santander, Bucaramanga, Colombia, 1995.
42. Consejo Superior de Investigaciones Científicas, Instituto de Estructura de la Materia, Madrid, España, 1995.
43. Departamento de Química Física Aplicada, Universidad Autónoma de Madrid, Madrid, España, 1995.
44. Departamento de Química y Física Teóricas, Consejo Superior de Investigaciones Científicas, Madrid, España, 1995.
45. Center for Theoretical Studies of Physical Systems, Clark Atlanta University, Atlanta, Georgia, USA, 1996.
46. The Royal Institution of Great Britain, London, UK, 1996.
47. Department of Chemistry, University of Bristol, Bristol, UK, 1996.
48. Institut für Organische Chemie, Technische Universität Dresden, Dresden, Germany, 1997.
49. Departamento de Química Física, Universidad de Santiago de Compostela, Santiago de Compostela, España, 1997.
50. Department of Chemistry and Biochemistry, University of Arkansas, Fayetteville, Arkansas, USA, 1998.
51. Department of Chemistry, Cornell University, Ithaca, New York, USA, 1998.
52. Facultad de Ciencias de la Computación, Benemérita Universidad Autónoma de Puebla, Puebla, México, 1998.
53. Institut für Organische Chemie, Technische Universität Dresden, Dresden, Germany, 1999.
54. "Graduierte Collegen" am der Institut für Organische Chemie, Technische Universität Dresden, Dresden, Germany, 1999.
55. Institut für Organische Chemie, Ruhr Universität, Bochum, Germany, 1999.
56. Institut für Organische Chemie, Universität Bremen, Bremen, Germany, 1999.
57. Institut für Physikalische und Theoretische Chemie, Friedrich - Alexander - Universität Erlangen-Nürnberg, Erlangen, Germany, 1999.
58. Grupo de Modelización Molecular, Instituto de Biotecnología, Universidad de Granada, Granada, España, 1999.
59. Instituto Central de Investigaciones de Matemática y Física (ICIMAF), Ministerio de Ciencias, Tecnología y Medio Ambiente, La Habana, Cuba, 1999.
60. Facultad de Ciencias, Universidad Industrial de Santander, Bucaramanga, Colombia, 2000.
61. Facultad de Química, Universidad Nacional de Colombia, Bogotá, Colombia, (February) 2000
62. Institut für Organische Chemie, Universität Bremen, Bremen, Germany, 2000.
63. Facultad de Química, Universidad Nacional de Colombia, Bogotá, Colombia, (November) 2000
64. Facultad de Agronomía, Universidad de Pinar del Río, Pinar del Río, Cuba, 2001.
65. Instituto Central de Investigaciones de Matemática y Física (ICIMAF), Ministerio de Ciencias, Tecnología y Medio Ambiente, La Habana, Cuba, 2001.
66. Facultad de Ciencias, Universidad de Granada, Granada, España, 2001.
67. Centro de Biofísica Médica, Universidad de Oriente, Santiago de Cuba, Cuba, 2002.
68. Centro de Investigaciones Biomédicas, Instituto Superior de Ciencias Médicas de La Habana, La Habana, Cuba, 2002.
69. Institut für Organische Chemie, Universität Bremen, Bremen, Germany, 2002.
70. Institut für Organische Chemie, Ruhr Universität, Bochum, Germany, 2002.
71. Institut de Química Computacional, Universitat de Girona, Girona, España, 2002.
72. Facultad de Química, Universidad de Barcelona, Barcelona, España, 2002.
73. Facultad de Química, Universidad Nacional de Colombia, Bogotá, Colombia, 2002.
74. Fundación Instituto de Inmunología de Colombia – FIDIC, Bogotá, Colombia, 2002.
75. Facultad de Biología, Universidad de La Habana, Havana, Cuba, 2003.
76. Centro Nacional de Sanidad Agropecuaria, San José de las Lajas, Cuba, 2003
77. Department of Chemistry, Oxford University, Oxford, UK, 2003.
78. Centre for Bioinformatics, Imperial College, London, UK, 2003.
79. The Wolfson Institute, University College of London, London, UK, 2003.
80. Institut für Organische Chemie, Universität Bremen, Bremen, Germany, 2003.
81. Institut für Organische Chemie, Ruhr Universität, Bochum, Germany, 2003.



82. Institut de Química Computacional, Universitat de Girona, Girona, España, 2003.
83. Facultad de Ciencias, Universidad de Cádiz, Cádiz, España, 2003.
84. Estación Experimental del Zaidín, CSIC, Granada, España, 2003.
85. Departamento de Química Física Aplicada, Universidad Autónoma de Madrid, Madrid, España, 2003.
86. The Wolfson Institute, University College of London, London, UK, 2003.
87. Faculty of Sciences, Université Henri Poincaré, Nancy, France, 2003.
88. Instituto de Ciencia Animal, Catalina de Güines, Cuba, 2003.
89. Department of Chemistry, Oxford University, Oxford, UK, 2004.
90. Facultad de Química, Universidad Nacional de Colombia, Bogotá, Colombia, 2004.
91. Fundación Instituto de Inmunología de Colombia – FIDIC, Bogotá, Colombia, 2004.
92. Facultad de Ciencias, Universidad de Extremadura, Badajoz, España, 2005.
93. Institut für Organische Chemie, Ruhr Universität, Bochum, Germany, 2005.
94. Departament d'Enginyeria Química, Escola d'Òptica i Optometria, Universitat Politècnica de Catalunya, Catalonia, España, 2005.
95. Departamento de Química Física Aplicada, Universidad Autónoma de Madrid, Madrid, España, 2005.
96. Facultad de Matemática y Computación, Universidad de La Habana, La Habana, Cuba, 2005.
97. Centro de Investigaciones de Materiales Avanzados, Chihuahua, México, 2005.
98. Facultad de Biología, Universidad de La Habana, La Habana, Cuba, 2006.
99. Institut für Organische Chemie, Ruhr Universität, Bochum, Germany, 2006.
100. Physical and Theoretical Chemistry Laboratories, The University of Oxford, Oxford, UK, 2006.
101. Dipartimento di Scienze Biochimiche, University of Rome "La Sapienza", Roma, Italia, 2006.
102. Universidad Autónoma de Ciudad Juárez, Ciudad Juárez, México, 2006.
103. *Laboratory of Ultrafast Spectroscopy, Institute of Chemical Sciences and Engineering (ISIC), EPFL, Lausanne, Suiza, 2007.*
104. *Laboratory of Computational Chemistry and Biochemistry, Institute of Chemical Sciences and Engineering (ISIC), EPFL, Lausanne, Suiza, 2007.*
105. Departamento de Química Física Aplicada, Universidad Autónoma de Madrid, Madrid, España, 2007.
106. Centro de Investigaciones de Materiales Avanzados, Chihuahua, México, 2007.
107. International Institute for the Study of Cuba, London, UK, 2007.
108. Institute of Ophthalmology of the University College of London, London, UK, 2007.
109. Faculdade de Ciências, Universidade de Lisboa, Lisboa, Portugal, 2008
110. Centre for Computational Science, University College of London, London, UK, 2008
111. Consejo Superior de Investigaciones Científicas, Instituto de Matemática y Física Fundamental, Madrid, España, 2008
112. Universidad Nacional de Colombia, Medellín, Colombia, 2008
113. Sede Universitaria de San Miguel del Padrón, Universidad de La Habana, Havana, 2009.
114. Institut für Organische Chemie, Ruhr Universität, Bochum, Germany, 2009.
115. Max-Planck-Institut für Kohlenforschung, Mülheim am Ruhr, Germany, 2009
116. Consejo Superior de Investigaciones Científicas, Instituto de Matemática y Física Fundamental, Madrid, España, 2009
117. Consejo Superior de Investigaciones Científicas, Instituto de Cerámica y Vidrio, España, 2009
118. Departamento de Química Física Aplicada, Universidad Autónoma de Madrid, Madrid, España, 2009.
119. Matemática Viva, Sociedad Cubana de Matemática, La Habana, 2009
120. Universidad de Chile, Departamento de Física, Santiago, Chile, 2010
121. Forschungszentrum Jülich GmbH, Jülich, Alemania, 2010
122. Institute of Labour Medicine, La Habana, Cuba, 2011
123. *Laboratory of Computational Chemistry and Biochemistry, Institute of Chemical Sciences and Engineering (ISIC), EPFL, Lausanne, Suiza, 2011.*
124. Departamento de Química, Universidade de Coimbra, Coimbra, Portugal, 2011.
125. Consejo Superior de Investigaciones Científicas, Instituto de Matemática y Física Fundamental, Madrid, España, 2011
126. University of Venda, Thohoyandou, Republic of South Africa, 2011.

127. College of Chemistry and Molecular Engineering, Peking University, Beijing, China, 2012
128. Dep. of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts, USA, 2012
129. David Rockefeller Center for Latin American Studies, Harvard University, Cambridge, Massachusetts, USA, 2012
130. Dep. of Chemistry, City College of New York, New York, USA, 2012
131. Dep. of Chemistry, University of Alabama, Tuscaloosa, USA, 2012
132. Dep. of Chemistry, University College of London, London, UK, 2013.
133. Centro de Estudios para el Perfeccionamiento de la Educación Superior, Universidad de La Habana, Havana, 2013.
134. Instituto Nacional de Oncología y Radiobiología, Havana, Cuba, 2013
135. Dep. of Chemistry, Federal University of Saõ Carlos, Saõ Carlos, Brasil, 2013.
136. Dep. of Pharmacy, Federal University of Rio de Janeiro, Rio de Janeiro, Brasil, 2013.
137. Dep. of Chemistry, Pontifical University of Rio de Janeiro, Rio de Janeiro, Brasil, 2013.
138. Donostia International Physics Center, Donostia, Basque Country, Spain, 2014
139. Departamento de Química Orgánica, Universidad Autónoma de Madrid, Madrid, Spain, 2014.
140. Facultad de Ciencias Químicas, Universidad Autónoma de Chihuahua, Chihuahua, Mexico, 2014
141. Universidad "Andrés Bello", Santiago de Chile, Chile, 2015
142. Institut für Organische Chemie, Ruhr Universität, Bochum, Germany, 2015
143. Department of Chemistry, University of Texas in El Paso, TX, USA, 2015
144. Departamento de Química, Universidade de Coimbra, Coimbra, Portugal, 2015.
145. Institute of Materials Sciences, University of Texas in Dallas, TX, USA, 2016
146. Universidad de Holguín, Holguín, Cuba, 2016
147. Johns Hopkins School of Medicine, Baltimore, MD, USA, 2016
148. Johns Hopkins University, Dep. of Chemistry, Baltimore, MD, USA, 2016
149. Dep. of Chemistry and Chemical Biology, Rutgers University, New Brunswick, NJ, USA, 2016
150. Dep. of Chemistry and Chemical Biology, Cornell University, Ithaca, NY, USA, 2016
151. Benemérita Universidad Autónoma de Puebla, Instituto de Física, Puebla, México, 2017
152. Universidad Nacional Autónoma de México, Instituto de Física, Ciudad de México, México, 2017
153. Universidad Central Marta Abreu de Las Villas, Santa Clara, Cuba, 2017
154. Universidad de Ciencias Informáticas, La Habana, Cuba, 2017
155. Facultad de Física de la Universidad de La Habana, La Habana, Cuba, 2018
156. Institut für Organische Chemie, Ruhr Universität, Bochum, Germany, 2018

**Graduate Courses:**

1. *Applications of computers to chemistry*, Centro Nacional de Investigaciones Científicas, La Habana, Cuba, 1974.
2. *Introduction to Computing Methods*, Universidad de La Habana, La Habana, Cuba, 1987, 1988, 1990.
3. *Molecular modeling*, Universidad de La Habana, La Habana, Cuba, 1992.
4. *Molecular modeling in personal computers*, Universitat de Girona, Girona, España, 1993.
5. *Molecular modeling in personal computers*, Universidad de Cádiz, Cádiz, España, 1993.
6. *Molecular modeling in personal computers*, Universitat de les Illes Balears, Palma de Mallorca, España, 1993.
7. *Molecular modeling in personal computers*, Universidad de Granada, Andalucía, España, 1993.
8. *Molecular modeling in personal computers*, Universidad Autónoma Metropolitana (Iztapalapa), México, D.F., 1993.
9. *Molecular modeling in personal computers*, Universidad de La Habana, La Habana, 1994.
10. *Molecular modeling in personal computers*, Universidad Nacional de Colombia, Santafe de Bogota, 1994.
11. *Advanced operating systems for PC's: Windows and Unix*, Universidad de La Habana, Facultad de Química, La Habana, yearly since 1994.
12. *Introduction to computational chemistry*, Universidad Nacional de Colombia, Medellín, 1997.
13. *Introduction to computational chemistry*, Facultad de Química, Universidad de La Habana, La Habana, 1998.
14. *Introduction to computational chemistry*, Instituto de Química, Universidad Mayor de San Andrés, La Paz, Bolivia, 2000.
15. *Introduction to computational chemistry*, Escuela de Química, Universidad Industrial de Santander, Bucaramanga, Colombia, 2000.
16. *Introduction to Linux operating system*, Escuela de Química, Universidad Industrial de Santander, Bucaramanga,

- Colombia, 2000.
17. *Introduction to Linux operating system*, Escuela de Matemática, Universidad Industrial de Santander, Bucaramanga, Colombia, 2000.
  18. *Introduction to Linux operating system*, Escuela de Química, Universidad Nacional de Colombia, Medellín, Colombia, 2000.
  19. *Molecular interactions*, Sonderforschungsbereich für supramolekulare Chemie, Universität Essen and Ruhr - Universität Bochum, Essen - Bochum, 2000
  20. *Introduction to computational chemistry*, Facultad de Ingeniería, Universidad Nacional de Colombia, Manizales, Colombia, 2001.
  21. *Introduction to computational chemistry*, Faculty of Sciences, Université Henri Poincaré, Nancy, France, 2003.
  22. *Introduction to computational chemistry*, Faculty of Chemical Sciences, Universidad Autónoma de Chihuahua, Chihuahua, México, 2005.
  23. *Introduction to computational chemistry*, Universidad Autónoma de Ciudad Juárez, Ciudad Juárez, México, 2006.
  24. *Introduction to molecular modelling*, Universidad de La Habana, La Habana, 2006.
  25. *Practical introduction to management of scientific literature: Endnote*, Centro de Investigaciones de Materiales Avanzados, Chihuahua, México, 2007.
  26. *Molecular interactions and computational chemistry*, Faculty of Chemical Sciences, Universidad Autónoma de Chihuahua, Chihuahua, México, 2007
  27. *Multiple Minima Hypersurfaces*, Universidad Nacional de Colombia, Medellín, 2008.
  28. *Introduction to molecular modelling*, University of Venda, Thohoyandou, Republic of South Africa, 2011.
  29. *Chem 253 - Modeling Matter at Nanoscales: An Introduction to Theoretical and Computational Approaches* (Fall 2012), Harvard University, Dep. of Chemistry and Biological Chemistry, Harvard University, Cambridge, Massachusetts, USA, 2012.
  30. *Modeling Matter at Nanoscales: An Introduction to Theoretical and Computational Approaches*, Dep. of Biology, Fluminense Federal University, Niteroi, Brasil, 2013.
  31. *Computational chemistry*, Faculty of Chemical Sciences, Universidad Autónoma de Chihuahua, Chihuahua, México, 2014
  32. *Computational Chemistry*, Faculty of Bioinformatics, Universidad de Talca, Talca, Chile, 2015
  33. *AS 030.407 - Modeling Matter at Nanoscales: An Introduction to Theoretical and Computational Approaches* (Fall 2016), Dep. of Chemistry, Johns Hopkins University, Baltimore, Maryland, USA, 2016.
  34. *Topics of Computational Chemistry*, Faculty of Bioinformatics, Universidad de Talca, Talca, Chile, 2018

#### **Documented Software:**

1. Montero, L.A. Alvarez, J.R., Del Bosque, J.R., **COPEANE**: *Cartesian Coordinates and Non Bonded Potentials*. Documented computer program for i-8086/8 processors under MS-DOS, Universidad de La Habana, 1986
2. Montero, L.A., **PPP**: *Molecular Orbitals and Excited States of Conjugated Molecules by the PPP Method*. Documented computer program for i-8086/8 processors under MS-DOS, Universidad de La Habana, 1986
3. Montero, L.A., Alvarez, J.R., Cano, R., González, M.C., **PCILO**: *Ground State Molecular Energy by Perturbative Configuration Interaction of Localized Orbitals*. Documented computer program for i-8086/8 processors under MS-DOS, Universidad de La Habana, 1986
4. Montero, L.A., Leonard, V., **MOLGRA**: *Molecular Graphics*. Documented computer program for i-8086/8 processors under MS-DOS, Universidad de La Habana, 1989
5. Montero, L.A., Alvarez, J.R., **MNDO**: *Molecular Orbitals and Optimized Geometries by the MNDO Method*. Documented computer program for i-8086/8 processors under MS-DOS, Universidad de La Habana, 1989
6. Montero, L.A., **NDOL**: *Molecular Orbitals and Excited States by SCF-NDO Methods*. Documented computer program for i-8086/8 processors under MS-DOS, Universidad de La Habana, 1989.
7. Montero, L.A., **ENHANCED MICROMOL**: *Molecular Orbitals, Optimized Geometries and Force Fields by ab initio SCF Methods*. Documented computer program for i-8086/8 processors under MS-DOS, Universidad de La Habana, 1989
8. Montero, L.A., **ICON**: *Molecular Orbitals by the Extended Hückel Theory*. Documented computer program for i-8086/8 processors under MS-DOS, Universidad de La Habana, 1989

9. Montero, L.A., **GEOMOL**: *Teaching to build Molecular Geometry Models*, Documented practical work and computer program for teaching how to build a molecular geometry model for i-8086/8 processors under MS-DOS, Universidad de La Habana, 1990.
10. Montero, L.A., Alvarez, J.R., **HAVPAC**: *Molecular Orbitals and Optimized Geometries by the MNDO, AM1 and PM3 Methods*. Documented computer program for i-8086/8 processors under MS-DOS, Universidad de La Habana, 1991.
11. Montero, L.A., **HAVMOL**: *Calculations of Molecular Structure and Properties by a Quantum Mechanical Approach, According to the ab initio SCF MO Theory of Roothaan*. Documented computer program for i-8086/386 processors under MS-DOS and MS-WINDOWS, Universidad de La Habana (Havana) and Consejo Superior de Investigaciones Científicas (Madrid), 1993.
12. Montero, L.A., Guevara, N., Mora, N., **NDOL32**: *Molecular Orbitals and Excited States by SCF-NDO Methods*. Version 3 for i386-Pentium processors, with enhanced input and output facilities and allowing up to 200 atoms, Technische Universität Dresden, Dresden, 1995 (Windows 95 and NT) and Universidad de La Habana, 1996 (Linux).
13. Montero, L.A., **MOPAC v.6**: *Semiempirical calculations of molecular properties by MNDO methods. Full implementation for i-386 and 486 computers of MOPAC v. 6*, Universidad de La Habana (Havana), 1994. Release 1.03, for Windows 95 and NT, and up to 200 atoms, 1997. Linux release, 1999.
14. Montero, L.A., **MOPAC v.7**: *Semiempirical calculations of molecular properties by MNDO methods. Full implementation for i-386, 486 and Pentium computers under Linux of MOPAC v. 7*, Universidad de La Habana (Havana), 1995.
15. Montero, L.A., Cruz, R., **MMH**: *Package of programs for processing data corresponding to multiple minima hypersurfaces of molecular clusters*, for MS-DOS, Universidad de La Habana e Instituto Superior de Ciencias y Tecnología Nuclear (Havana), 1997 and 2000. Documented in <http://karin.fq.uh.cu/mmh/>.
16. Montero, L.A., **NDOL2000**: *Molecular Orbitals and Excited States by SCF-NDO Methods*. Version 3.1 for i386-Pentium processors, with enhanced input and output facilities and allowing more than 200 atoms, Universidad de La Habana, 2000 (Windows systems).
17. Montero, L.A., **NDOL2004**: *Molecular Orbitals and Excited States by SCF-NDO Methods*. Version 3.95 for i386-Pentium processors, with enhanced input and output facilities and allowing more than 300 atoms and 800 basis orbitals, Universidad de La Habana, 2004 (Windows systems).
18. Montero, L.A., **MOPAC6J**: *Semiempirical calculations of molecular properties by MNDO methods. Full implementation for i-386 and 486 computers of MOPAC v. 6 including the new Jorgensen Hamiltonians and MMH facilities*, Universidad de La Habana (Havana), 2004. for Windows and Linux.
19. Montero, L.A., **NDOL2007**: *Molecular Orbitals and Excited States by SCF-NDO Methods*. Version 5 for i386-Pentium processors, with enhanced input and output facilities and allowing more than 300 atoms and 800 basis orbitals, Universidad de La Habana, 2007 (Windows systems).
20. Montero, L.A., **NDOL2008**: *Molecular Orbitals and Excited States by SCF-NDO Methods*. Version 6 for i386-Pentium processors, with enhanced input and output facilities and allowing more than 400 atoms and 800 basis orbitals, and full single configuration interactions. Universidad de La Habana and Universidad Autónoma de Madrid, 2008 (Windows and Linux systems).
21. Montero, L.A., **NDOL2009**: *Molecular Orbitals and Excited States by SCF-NDO Methods*. Version 6.6 for i386-Pentium processors, with enhanced input and output facilities and dynamic memory allocation to allowing very large systems depending on computer availability. Universidad de La Habana and Universidad Autónoma de Madrid, 2009 (Linux systems).
22. Montero, L.A., **NDOL2010**: *Molecular Orbitals and Excited States by SCF-NDO Methods*. Version 6.7 for i386-Pentium processors, with enhanced SCF convergence criteria and facilities for batch calculations on different structures of the same system. Universidad de La Habana and Universidad Autónoma de Madrid, 2010 (for both Windows and Linux systems). Copyrighted in Havana.
23. Montero, L.A., **NDOL2015**: *Molecular Orbitals and Excited States by SCF-NDO Methods*. Version 7.0.3 with more rich SCF convergence menu and facilities to map electron densities corresponding to different excited states. Universidad de La Habana, 2015 (for both Windows and Linux systems). Copyrighted in Havana.

**Participation in funded projects for research:**

*Title:* Física teórica de moléculas

*Funding entity:* Consejo Superior de Investigaciones Científicas, Madrid, España

*Lasting time:* 1987 to 1990

*Main researchers:* Luis A. Montero and Yves G. Smeyers (Consejo Superior de Investigaciones Científicas, Madrid, España)

*Title:* Theoretical Chemistry in Personal Computers: Creation and Education.

*Funding entity:* Swedish Agency for Research Cooperation with Developing Countries (SAREC), Stockholm, Sweden.

*Lasting time:* 1991 to 1994

*Main researchers:* Sten Lunnell (Uppsala University, Sweden) and Luis A. Montero

*Title:* Theoretical Chemistry

*Funding entity:* Deutsche Akademischer Austauschdienst (DAAD), Bonn, Germany.

*Lasting time:* 1996 to 1997

*Main researcher:* Luis A. Montero

*Title:* Diseño y Modelación de Procesos Moleculares de Interés Biológico y Ambiental.

*Funding entity:* Ministerio de Ciencias, Tecnología y Medio Ambiente, La Habana, Cuba.

*Lasting time:* 1995 to 1998

*Main researcher:* Luis A. Montero

*Title:* Partnership for the use of personal computers and clusters of PC's in computational chemistry

*Funding entity:* Deutsche Akademischer Austauschdienst (DAAD), Bonn, Germany.

*Lasting time:* 2002 to 2005

*Main researchers:* Luis A. Montero and Wolf-Dieter Stohrer (University of Bremen, Germany)

*Title:* Synthesis, immobilisation and electrochemical characterization of metalloporphyrinoids for catalysis, as sensors and for light induced electron transfer

*Funding entity:* Deutsche Forschungsgemeinschaft

*Lasting time:* 2006 to 2008

*Main researchers:* Franz-Peter Montforts (University of Bremen, Germany) and Luis A. Montero

*Title:* Conformations and associations of carbohydrates – computation and experiment

*Funding entity:* The Royal Society of Great Britain

*Lasting time:* 2007 to 2008

*Main researchers:* Lavina Snoek (University of Oxford, UK) and Luis A. Montero

*Title:* Virtual Center of Bioinformatics, Scientific Education and Creation

*Funding entity:* Spanish Agency of International Cooperation for Development

*Lasting time:* 2009 to 2012

*Main researchers:* José M. García de la Vega (Spain) and Luis A. Montero

*Title:* Estados electrónicos de grafenos, nanotubos de carbono, fullerenos y nanocristales con posibles dopantes

*Funding entity:* Universidad Autónoma de Madrid and Banco Santander

*Lasting time:* 2009 to 2010

*Main researchers:* José M. García de la Vega (Spain) and Luis A. Montero

*Title:* Avaliação dos produtos naturais bioativos de organismos marinhos com potencial uso no tratamento de doenças infecciosas

*Funding entities:* CAPES and MES-CUBA

*Lasting time:* 2013 - 2015

*Main researchers:* Valeria Laneuville Teixeira (Brasil) and Luis A. Montero

Title: Racionalización de la regioselectividad y la estereoselectividad de reacciones orgánicas empleadas en "Click Chemistry" en ausencia de catalizadores

*Funding entities:* CITMA and MES-CUBA

*Lasting time:* 2013 - 2016

*Main researchers:* Luis A. Montero

Title: Densidades electrónicas de excitones nanoscópicos. Posibles aplicaciones fotofísicas y fotoquímicas

*Funding entities:* CITMA and MES-CUBA

*Lasting time:* 2018 - 2021

*Main researchers:* Luis A. Montero

Title: Diseño *in silico* de nanopartículas portadoras de protoporfirina ix para la terapia fotodinámica del cáncer

*Funding entities:* CITMA and MES-CUBA

*Lasting time:* 2018 - 2021

*Main researchers:* Luis A. Montero

Title: Modelación teórica de la relación Estructura/Actividad del antibiótico Tirocidina A y sus análogos: Un camino en la búsqueda de fármacos novedosos.

*Funding entities:* CITMA and MES-CUBA

*Lasting time:* 2018 - 2021

*Main researchers:* Luis A. Montero

***Long stays in foreign intitutions (longer than 4 weeks):***

1. Sektion Chemie. Technische Universität Dresden, Dresden, Germany, 1980, 4 months, Theoretical chemistry. Doctorate degree.
2. Dirección de Investigaciones. Consejo Nacional de la Educación Superior, Managua, Nicaragua, 1982, 2 months, Science policy. Invited advisor.
3. Sektion Chemie. Technische Universität Dresden, Dresden, Germany, 1986, 2 months, Theoretical chemistry. Postdoctoral fellowship.
4. Institut of Quantum Chemistry. Uppsala University, Uppsala, Sweden, 1991, 1 month, Theoretical chemistry. Academic exchange.
5. Instituto de Estructura de la Materia. Consejo Superior de Investigaciones Científicas (CSIC), Madrid, Spain, 1992-93, 1 year, Theoretical chemistry. Sabatical.
6. Institut für Organische Chemie. Technische Universität Dresden, Dresden, Germany, 1995, 3 months, Theoretical chemistry. Postdoctoral fellowship.
7. Grupo de Modelización Molecular, Instituto de Biotecnología. Universidad de Granada, Granada, Spain, 1996, 1 month, Theoretical chemistry. Invited professorship.
8. Institut für Organische Chemie. Technische Universität Dresden, Dresden, Germany, 1999, 2 months, Theoretical chemistry. Postdoctoral fellowship.
9. Lehrstuhl für Physikalische und Theoretische Chemie. Universität Erlangen - Nürnberg, Erlangen, Germany, 1999, 1 month, Theoretical chemistry. Postdoctoral fellowship.
10. Facultad de Ciencias, Universidad Industrial de Santander, Bucaramanga, Colombia, 2000. 1 month. Invited professorship.
11. Lehrstuhl für Organische Chemie 2, Ruhr-Universität Bochum, Bochum, Germany, 2000. 1 month. Invited professorship.
12. Davy Faraday Research Laboratory, The Royal Institution of Great Britain, London, UK, 2000, 1 month, Invited researcher.
13. Institut für Organische Chemie. Universität Bremen, Bremen, Germany, 2002, 1 month, Theoretical chemistry. Invited professorship.
14. Davy Faraday Research Laboratory, The Royal Institution of Great Britain, London, UK, 2003, 1 month, Invited

researcher.

15. Institut für Organische Chemie. Universität Bremen, Bremen, Germany, 2003, 1 month, Theoretical chemistry. Invited professorship.
16. Institut für Organische Chemie. Universität Bremen, Bremen, Germany, 2004, 1 month, Theoretical chemistry. Invited professorship.
17. Department of Chemistry, University of Oxford, Oxford, UK, 2004, 1 month, Theoretical chemistry, Invited professorship.
18. Departamento de Química Física Aplicada, Facultad de Ciencias, Universidad Autónoma de Madrid, Madrid, Spain, 2005, 3 months, Theoretical and computational chemistry, visiting professorship.
19. Institut für Organische Chemie. Universität Bremen, Bremen, Germany, 2006, 1 month, Theoretical chemistry. Invited professorship.
20. *Laboratory of Ultrafast Spectroscopy, Institute of Chemical Sciences and Engineering (ISIC), EPFL, Lausanne, Switzerland, 2007, 1 month. Theoretical chemistry. Invited professorship.*
21. Departamento de Química Física Aplicada, Facultad de Ciencias, Universidad Autónoma de Madrid, Madrid, Spain, 2008, 3 months, Theoretical and computational chemistry, visiting professorship.
22. Lehrstuhl für Organische Chemie 2, Ruhr-Universität Bochum, Bochum, Germany, 2009. 1 month. Invited professorship.
23. Departamento de Química Física Aplicada, Facultad de Ciencias, Universidad Autónoma de Madrid, Madrid, Spain, 2009, 1 month, Theoretical and computational chemistry, visiting professorship.
24. Departamento de Química Física Aplicada, Facultad de Ciencias, Universidad Autónoma de Madrid, Madrid, España, 2010, 1 month, Theoretical and computational chemistry, visiting professorship.
25. Departamento de Química Física Aplicada, Facultad de Ciencias, Universidad Autónoma de Madrid, Madrid, España, 2011, 1 month, Theoretical and computational chemistry, visiting professorship.
26. Departamento de Química Física Aplicada, Facultad de Ciencias, Universidad Autónoma de Madrid, Madrid, España, 2012, 1 month, Theoretical and computational chemistry, visiting professorship.
27. David Rockefeller Center for Latin American Studies and Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts, USA, Sept. – Dec. 2012, Santander Visiting Scholar.
28. Dep. of Biology, Fluminense Federal University, Niteroi, Brasil, November, 2013, Visiting Professor.
29. Dep. of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts, USA, February, 2014, visiting professor
30. Donostia International Physics Center, Donostia, Basque Country, Spain, June – July, 2014, invited professor.
31. Departamento de Química, Universidade de Coimbra, Coimbra, Portugal, November – December, 2015, invited professor.
32. Dep. of Chemistry, Johns Hopkins University, Baltimore, Maryland, USA, 2016. Professor visitante.