

# CURRICULUM VITAE

## Adélia Justina Aguiar Aquino

### 1. Personal Information

*Name:* Adélia Justina Aguiar Aquino

*Citizenship:* Brazil

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### 2. Education

- Ph.D. Chemistry, Universidade de São Paulo, Brazil, 1991.  
Thesis: An ab-initio study of the molecules  $P_2O$ ,  $P_2O^+$ ,  $N_2S$  and  $N_2S^+$   
advisor: Fernando Rei Ornellas
- M.S. Chemistry, Universidade de São Paulo, Brazil, 1984.  
Thesis: Studies on the polythiazil polymer using molecular orbital theory  
advisor: Milan Trsic
- Teaching Credentials Chemistry, Universidade de Brasília, Brazil, 1982.
- B.S. Chemistry, Universidade de Brasília, Brazil, 1979.

### 3. Career History

Scientific Development Analyst of the CNPq (National Council of Scientific and Technological Development) Brasília, Brazil (1981-1984)

Chemistry Program Supervisor at the CNPq (1985-1993)

Associate Research, Phys. Depart., University of Brasilia, Brazil (1991-1993)

Postdoc, Physics. Department, University of California, San Diego and San Diego Computer Center, La Jolla, CA, USA (1994-1997)

Program coordinator for the division of Biological and Environmental Sciences at CNPq, Brasília, Brazil (1997-1999)

Management and scientific position in the international collaboration project Brazil x Austria, Organic matters in tropical soils, Austrian Research Centers and the University of Vienna (1999-2002)

Program Officer, United Nations Office for Outer Space Affairs (UN-OOSA), Vienna, Austria (2003)

Researcher at the Institute of Theoretical Chemistry, University of Vienna in the framework of the Advanced Light Sources (ADLIS) program (2004)

Senior Researcher in a joint proposal between the University of Vienna, University of Natural Resources and Applied Sciences, Vienna and Austrian Institute of Technology (AIT) (2005-2013)

Research Professor at the Depart. of Chem. and Biochem. Texas Tech University (TTU), Lubbock, Texas, USA (2011- 2015)

Professor at the School of Pharmaceutical Science and Technology, Tianjin University, Tianjin, China (2015 – 2019)

Adjunct Professor Depart. of Chem. and Biochem. Texas Tech University (TTU), Lubbock, Texas, USA (2015 - )

Short-term professor position -Tianjin University, Tianjin China (2019- )

Associate Professor of Practice at the Department of Mechanical Engineering, TTU, Lubbock, TX, USA (2019-)

#### 4. Professional Societies

- Sociedade Brasileira de Química (Brazilian Chemistry Society)
- American Chemical Society

#### 5. Member of the organization committees of academic activities

##### a) *Symposia*

Recent Developments in Computational Chemistry – Can Theory Answer Questions on Applied Natural Sciences? 27 June 2003, University of Natural Resources and Applied Life Sciences, Vienna, Austria

Electron correlation and molecular dynamics for excited states and photochemistry, 3-4 July 2008, Erwin Schrödinger Institute, Vienna

DFG-IUSS SYMPOSIUM - Advances of Molecular Modeling of Bio-Geo-Chemical Interfaces– Perspectives for Soil Research, 6-7 October 2009, Jena, Germany

##### b) *Schools*

COLUMBUS in RIO: A Quantum Chemistry Course on Multireference Methods, Energy Surfaces, Excited States and Dynamics, November 27 – December 2, 2005 Instituto Militar de Engenharia (IME) Rio de Janeiro – Brazil.

COLUMBUS in Bangkok: A Multireference Methods Workshop - The 3rd Thai Summer School of Computational Chemistry, Apr. 2 - 5, 2006, Burapha University, Bang Saen, Thailand Mixed Quantum-Classical Dynamics: Foundations and Application to Photo-Biological Questions, summer school July 7-12, 2008, University of Vienna, Vienna, Austria.

Mixed Quantum-Classical Dynamics: Foundations and Application to Photo-Biological Questions, Summer School July 7-12, 2008, University of Vienna, Vienna, Austria.

COLUMBUS in China - An Advanced Quantum Chemistry Workshop on Multireference Methods, Energy Surfaces, Polyradical Systems, Excited States and Dynamics, Oct 10-14, 2016, School of Pharmaceutical Sciences and Technology Tianjin University Tianjin – China

#### 6. Conferences and Meetings Attended

I have attended more than hundred conferences, workshops and seminars. I gave invited talk in forty of them.

#### 7. Publications

Currently 137 publications in peer-reviewed journal and 7 book chapters.

#### 8. Research Interest

Computer simulations based on quantum chemical methods applied to energy, renewable energy, biological and environmental related fields: i) modeling basic interactions in molecular models of humic substances such as nanopores and wet regions; ii) the interaction between mineral surfaces and different organic compounds; iii) modeling of defect transport in DNA; iv) excited-state proton transfer; v) modeling of graphene defects; vi) organic photovoltaic processes; vii) spectroscopic properties and solvent effect of natural pigments; viii) combustion reactions on different mineral surfaces; and ix) electron transfer reaction in the catalytic cycle of cytochrome P450 enzymes.