

## BIOGRAPHICAL SKETCH, Adelia Aquino

### (a) Professional Preparation

- |                           |           |                           |
|---------------------------|-----------|---------------------------|
| • University of Brasília  | Chemistry | Bachelor, 1979            |
| • University of Brasília  | Chemistry | Teaching Credential, 1981 |
| • University of São Paulo | Chemistry | Master, 1984              |
| • University of São Paulo | Chemistry | Ph.D., 1991               |

### (b) Appointments

- Associated Professor of Practice, Department of Mechanical Engineering, Texas Tech University, Lubbock, TX (2019 – present)
- Professor, short term contract, School of Pharmaceutical Science and Technology, Tianjin University (TJU), Tianjin, China (2019-2021)
- Professor, School of Pharmaceutical Science and Technology, Tianjin University (TJU), Tianjin, China (2015-2019)
- Adjunct Professor, Depart. of Chem. and Biochem., Texas Tech University (TTU), Lubbock, Texas, USA. (2015-present)
- Research Professor at the Depart. Chem. and Biochem., Texas Tech University (TTU), Lubbock, Texas, USA. (2011-2015)
- Senior Scientist in a joint proposal between the Univ. of Vienna (Univie), the Univ. of Natural Resources and Applied Sciences, Vienna, and the Austrian Research Centres, Seibersdorf (2005-2010)
- Senior Scientist at the Institute of Theor. Chem. of Univie in the framework of the ADvanced Light Sources (ADLIS) research program (2004)
- Programme Officer, United Nations Office for Outer Space Affairs (UN-OOSA), Vienna, Austria (2003)
- Management and scientific position in an international collaboration project Brazil x Austria, “Organic Matters in a Tropical Soils”, at the Austrian Research Centers, Seibersdorf and the Univ. of Vienna (1999-2002)
- Coordinator, division of Biol. and Environ. Sci. at the National Council for Scientific and Technological Develop. (CNPq), Brasília, Brazil (1997-1998).
- Postdoctoral program at the Phys. Depart., Univ. California, San Diego and the San Diego Supercomputer Center (1994-1996).
- Coordinator of Human Resources for Strategic Areas (RHAE) and technical secretary of subprogram Chem. and Chem. Eng. (QEQ) at CNPq in the framework of the Program for Support of Scientific. and Technological Development (PADCT) (1990-1993)
- Chemistry Program Supervisor at CNPq (1985-1989)
- Scientific and Technological Development Analyst at CNPq, (1981-1984)

### (c) Ten significant publications

1. Adelia J.A. Aquino, Daniel Tunega, Georg Haberhauer, Martin H. Gerzabek and Hans Lischka "Solvent effects on hydrogen bonds - A theoretical study" *J. Phys. Chem.*, **106** (2002) 1862-1871.
2. Adelia J.A. Aquino, H. Lischka, and C. Hattig, “Excited-state intramolecular proton transfer: A survey of TDDFT and RI-CC2 excited-state potential energy surfaces” *J. Phys. Chem. A* 109 (2005) 3201-3208.
3. Adelia J.A. Aquino, D. Tunega, G. Haberhauer, M. H. Gerzabek and H. Lischka “Acid-base properties of a goethite surface model: a theoretical view”, *Geochimica et Cosmochimica Acta*, **72** (2008) 3587-3602.
4. Adelia J.A. Aquino, Daniel Tunega, Gabriele E. Schaumann, Georg Haberhauer, Martin H. Gerzabek, and Hans Lischka “Stabilizing Capacity of Water Bridges in

- Nanopore Segments of Humic Substances: A Theoretical Investigation” *J. Phys. Chem. C* **113** (2009)16468-16475.
5. Mario Barbatti, Adélia J.A. Aquino and Hans Lischka. “The UV absorption of nucleobases: semi-classical ab initio spectra simulations” *Phys. Chem. Chem. Phys.* **12** (2010) 4959-4967.
  6. Adelia J.A. Aquino, D. Nachtigallova, P. Hobza, D.G. Truhlar, C. Hattig, H. Lischka, “The Charge-Transfer States in a Stacked Nucleobase Dimer Complex: A Benchmark Study” *J. Comp. Chem.* **32** (2011) 1217-1227.
  7. Adelia J.A. Aquino, Daniel Tunega, Hasan Pasalic, Gabriele E. Schaumann, Georg Haberhauer, Martin H. Gerzabek and Hans Lischka, “Molecular dynamics simulations of water molecule-bridges in polar domains of humic acids” *Environmental Science & Technology* **45** (2011) 8411-8419.
  8. Adelia J.A. Aquino, D. Tunega; G. E. Schaumann, Georg Haberhauer, M. H. Gerzabek, H. Lischka, “The Functionality of Cation Bridges for Binding Polar Groups in Soil Aggregates” *Intern. J. Quantum Chem.* **111** (2011) 1531-1542.
  9. “Density Functional Theory Analysis Identifying the Mechanism for Ignition Sensitivity of Ammonium Periodate Compared with Ammonium Perchlorate” A. de Rezende, M.L. Pantoya, D. Tunega, B. Fuchs, A.R. Demko, Adelia J.A. Aquino, *J. Phys. Chem. C*, **126**, (2022), 21723–21733.
  10. “Machine Learning for Designing Mixed Metal Halides for Efficient Ammonia Separation and Storage” A. de Rezende, M. Malmali, P.O. Dral, H. Lischka, H. D. Tunega, Adelia J.A. Aquino, *J. Phys. Chem. C*, **126** (2022) 2184-2196.

(d) Synergistic Activities

1. Chemistry Program Supervisor at CNPq, Brasília, Brazil (1985-1989)
2. In CNPq, coordinator of Human Resources for Strategic Areas (RHAE) and technical secretary of subprogram Chem. and Chem.l Eng. (QEQ) in the framework of the Program for Support of Scient. and Techn. Develop.(PADCT) (1990-1993)
3. Coordinator, division of Biol. and Environ. Sc. at CNPq (1997-1998).
4. Member of the organizing committees of the following events: i) Recent Develop. in Comp. Chem. – Can Theory Answer Questions on Applied Natural Sciences? 27 June 2003, Vienna, Austria; ii) Electron correlation and molecular dynamics for excited states and photochemistry, 3-4 July 2008, Vienna; iii) Advances of Molecular Modelling of Bio-Geo-Chemical Interfaces-Perspectives for Soil Research 6-7 of October 2009, Jena, Germany.
5. Member of the organizing committees of seasonal schools:  
 COLUMBUS in Rio: Course on Multireference (MR) Methods, Nov. 27 – Dec. 2, 2005, Rio de Janeiro, Brazil; COLUMBUS in Bangkok: A MR Methods Workshop, Apr. 2 - 5, 2006, Bang Saen, Thailand; Summer School, Mixed Quantum-Classical Dynamics, July 7-12, 2008, Vienna, Austria

(e) Collaborators & Other Affiliations

- Collaborators and Co-Editors

Michelle Pantoya, Clemens Krempner, Carol Korzeiniewski, Moira Ridley, Bill Poirier, Yehia Mechref, Mahdi Malmali, Guigen Li – TTU, USA; Irene Burghardt (Goethe-University, Germany), Daniel Tunega, Martin Gerzabek - Univ. of Natural Resources and Applied Life Sciences, Vienna; Ivelina Georgieva (Bulgarian Acad. of Sci., Bulgaria), Dana Nachtigallova (Czech Acad. of Sci. Czech Republic), Itamar Borges (Instituto Militar de Engenharia, Rio de Janeiro, Brazil), Francisco Bolivar Correto Machado (Inst. Tecnológico de Aeronáutica, São Paulo, Brazil), Mario Barbatti (Aix-Marseille Université, Marseille, France), Han Zuilhof (Wageningen University, the Netherlands)

- Current graduate students: one masters, three PhD; five undergrad students; over 180 academic publications in refereed journals, and 5 book chapters.