

Ivan Tubert-Brohman

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Education

Ph. D. in Computational Chemistry, 2001–2006. Dissertation topic: *The development of improved semiempirical methods*; Research Advisor: William L. Jorgensen
Yale University

M. Sc. in Organic Chemistry, 2001–2002
Yale University

B.Sc. in Chemistry, 1995–2001. Undergraduate thesis: *Computer-Assisted Organic Synthesis: Development of an Educational Software Package*; Thesis Advisor: José Manuel Méndez-Stivalet
National Autonomous University of Mexico

Overall GPA: 9.86/10

Exchange student, 1998. Education Abroad Program
University of California at Berkeley

Job history

Senior Scientist

Schrodinger, LLC

2009–Present

Research and development of computational chemistry software with applications to pharmaceutical research.

Postdoctoral fellow

University of Basel

2007–2008

Worked with Prof. Markus Meuwly on methods for the simulation of transition-metal catalyzed hydrogenation reactions and reactive molecular dynamics applied to proton transfer in ferredoxins.

Postdoctoral fellow

Harvard University

2006–2007

Worked with Prof. Alan Aspuru-Guzik on distributed computing applications for clean energy materials and quantum computing algorithms for protein folding.

Honors, Fellowships, and Awards

- **Marie Curie Incoming International Fellowship**, The European Commission, 2007–2008
Fellowship for postdoctoral research at the University of Basel under Prof. Markus Meuwly
- **Richard Wolfgang Prize**, Yale University, 2007
Best dissertation in Chemistry
- **CINF Scholarship for Scientific Excellence**, ACS Division of Chemical Information, sponsored by IO Informatics, 2005
230th ACS National Meeting, Washington, DC
- **CCG Excellence Award**, ACS Division of Computers in Chemistry and the Chemical Computing Group., 2004
227th ACS National Meeting, Anaheim, California
- **Gabino Barrera medal**, National Autonomous University of Mexico, 2001
Given to the top student of each class
- **Telmex Fellowship**, Telefonos de Mexico, 1997-1999
Given by the national phone company by national competition
- **Second place**, 2nd Inter-university Math Contest (Mexico City), 1998
- **Gold medal**, Iberoamerican Chemistry Olympiad (Buenos Aires), 1995
- **Silver medal**, International Chemistry Olympiad (Beijing), 1995
- **Bronze medal**, International Chemistry Olympiad (Oslo), 1994

Past and current Research Interests

- Modeling of asymmetric hydrogenation reactions. Developed a force field for the simulation of iridium complexes used as catalysts for asymmetric hydrogenation reactions.
- Electron-coupled proton transfer. Developed and applied a molecular-mechanics proton transfer algorithm to the electron-coupled proton transfer in *Azotobacter Vinelandii* Ferredoxin I.
- Virtual screening. Used genetic algorithms to optimize a chemical similarity search protocol for the search of HIV non-nucleoside reverse transcriptase inhibitors.
- QM/MM simulation of enzymatic reactions. Applied Monte Carlo quantum mechanical/molecular mechanical simulations to reactions catalyzed by chorismate mutase, halohalkane dehalogenase, fatty acid amide hydrolase, and artificially designed proteins.
- Steric effects on acidity. Studied steric and solvent effects on pKa via density functional theory combined with Monte Carlo statistical mechanical simulations.
- Semiempirical quantum molecular orbital methods. Developed improved semiempirical methods by using statistical bond and group equivalents, by modifying the core repulsion function, and by introducing orthogonalization corrections to the SCF calculation.
- Computer-assisted organic synthesis. Designed and implemented a client-server Computer-Assisted Organic Synthesis system, which includes pattern recognition, a language interpreter, a graphical user interface, and a knowledge base.

Publications

- Tubert-Brohman, I.; Schmid, M.; Meuwly, M. "Molecular mechanics force field for octahedral organometallic compounds with inclusion of the trans influence". *J. Chem. Theory Comput.* 2009. 5. 530-539. <http://dx.doi.org/10.1021/ct800392n>.
- Perdomo, A.; Truncik, C.; Tubert-Brohman, I.; Rose, G.; Aspuru-Guzik, A. "Construction of model Hamiltonians for adiabatic quantum computation and its application to finding low energy conformations of lattice protein models". *Phys. Rev. A* 2008. 78. 012320. <http://dx.doi.org/10.1103/PhysRevA.78.012320>.
- Barreiro, G.; Guimaraes, C. R. W.; Tubert-Brohman, I.; Lyons, T. M.; Tirado-Rives, J.; Jorgensen, W. L. "Search for Non-Nucleoside Inhibitors of HIV-1 Reverse Transcriptase Using Chemical Similarity, Molecular Docking, and MM-GB/SA Scoring". *J. Chem. Inf. Model.* 2007. 47. 2416-2428. <http://dx.doi.org/10.1021/ci700271z>.
- Tubert-Brohman, I.; Acevedo, O.; Jorgensen, W. L. "Elucidation of Hydrolysis Mechanisms for Fatty Acid Amide Hydrolase and Its Lys142Ala Variant via QM/MM Simulations". *J. Am. Chem. Soc.* 2006. 128. 16904-16913. <http://dx.doi.org/10.1021/ja065863s>.
- Sattelmeyer, K.; Tubert-Brohman, I.; Jorgensen, W. L. "NO-MNDO: Reintroduction of the Overlap Matrix into MNDO". *J. Chem. Theory Comput.* 2006. 2. 413-419. <http://dx.doi.org/10.1021/ct050174c>.
- Tubert-Brohman, I.; Guimaraes, C. R. W.; Jorgensen, W. L. "Extension of the PDDG/PM3 Semiempirical Molecular Orbital Method to Sulfur, Silicon, and Phosphorus". *J. Chem. Theory Comput.* 2005. 1. 817-823. <http://dx.doi.org/10.1021/ct0500287>.
- Guimaraes, C. R. W.; Udier-Blagovic, M.; Tubert-Brohman, I.; Jorgensen, W. L. "Effects of Arg90 Neutralization on the Enzyme-Catalyzed Rearrangement of Chorismate to Prephenate". *J. Chem. Theory Comput.* 2005. 1. 617-625. <http://dx.doi.org/10.1021/ct0500803>.
- Tubert-Brohman, I. "Annotating CPAN". *perl.com*. June 2004. <http://perl.com/pub/a/2005/06/30/annocpan.html>.
- Tubert-Brohman, I. "Perl and Chemistry". *The Perl Journal*. June 2004. 6. 3-5. <http://www.tpj.com/documents/s=9607/tpj0406/>.
- Tubert-Brohman, I.; Guimaraes, C. R. W.; Repasky, M. P.; Jorgensen, W. L. "Extension of the PDDG/PM3 and PDDG/MNDO Semiempirical Molecular Orbital Methods to Halogens". *J. Comput. Chem.* 2004. 25. 138-150. <http://dx.doi.org/10.1002/jcc.10356>.
- Tubert-Brohman, I.; Talanquer, V. "Sobre adsorción. [About Adsorption.]". *Educación Química*. 1997. 8. 186-190.

Presentations

- Tubert-Brohman, I.; Schmid, M.; Meuwly, M. "A molecular mechanics force field for octahedral organometallic compounds with inclusion of the trans influence". *American Chemical Society Fall National Meeting (also presented at the International Conference on Organometallic Chemistry and the Swiss Chemical Society National Meeting)*. 2008.
- Tubert-Brohman, I.; Acevedo, O.; Jorgensen, W. L. "Elucidation of Hydrolysis Mechanisms for Fatty Acid Amide Hydrolase and Its Lys142Ala Variant via QM/MM Simulations". *Swiss Chemical Society National Meeting*. 2007.
- Tubert-Brohman, I. "Elucidation of Hydrolysis Mechanisms for Fatty Acid Amide Hydrolase and Its Lys142Ala Variant via QM/MM Simulations". *AMGEN*. 2006.

- Tubert-Brohman, I.; Jorgensen, W. L. "Mok - A domain-specific language for molecular information processing". *American Chemical Society 230th National Meeting. Washington, DC.* 2004.
- Tubert-Brohman, I. "PDDG/PM3: an Improved Semiempirical Molecular Orbital Method.". *Club Med Seminar. Yale University.* 2004.
- Tubert-Brohman, I.; Guimaraes, C. R. W.; Jorgensen, W. L. "Improved Semiempirical Methods: Parameterization of PDDG/PM3 for Sulfur". *American Chemical Society 227th National Meeting. Anaheim, CA.* 2004.
- Tubert-Brohman, I.; Guimaraes, C. R. W.; Repasky, M. P.; Jorgensen, W. L. "PDDG/PM3 and PDDG/MNDO: Extension to the Halogens". *American Chemical Society 226th National Meeting. New York.* 2003.
- Tubert-Brohman, I.; Repasky, M. P.; Jorgensen, W. L. "Semiempirical Heats of Formation through the use of Bond and Group Equivalents--Extension to the Halogens". *Third Metropolitan Area Poster Program for Graduate Students in Chemical Sciences. American Chemical Society, New York Section.* 2003.
- Tubert-Brohman, I.; Mendez-Stivalet, J. M. "Síntesis Orgánica Asistida por Computadora: Desarrollo de un programa educativo". *Congreso Nacional de Química. San Luis Potosí, Mexico.* 2001.

Teaching Experience

Math and Science Tutor

Yale University
2004–2006

Helped the students of Yale's Calhoun College with problems in Chemistry, Physics, and Calculus.

Teaching Fellow

Yale University
2001–2004

Computational Chemistry (1 semester), Organic Chemistry (2 semesters), and Organic Chemistry Lab (2 semesters). Responsibilities included leading a lab and/or discussion section and grading.

Teaching Assistant

National Autonomous University of Mexico
2000–2001

Physical Chemistry (1 semester) and Heterocyclic Organic Chemistry (1 semester). Responsibilities included lecturing, leading a lab and a discussion section and grading.

Mentor, Mexican Chemistry Olympiad

National Autonomous University of Mexico
1996–2001

Participated in the training of the teams from Mexico City and Oaxaca, as well as a mentor of the national delegation to the Iberoamerican Chemistry Olympiad in Venezuela in 2000. Worked in design and grading of exams, logistics, website design and administration.

Computer Skills

Languages: Perl (expert), C (advanced), Fortran (intermediate), JavaScript (intermediate), VBA (basic), 8086 Assembler (basic), Java (basic).

Web-related technologies: HTML, XML, CSS, mod_perl, Apache.

Version Control: CVS, Subversion, Perforce, VSS.

Operating systems: Linux, Irix, Windows.

Scientific software: Gaussian, MOPAC, CHARMM, BOSS, JMP, Matlab.

Open Source Software Development Experience (volunteer projects)

PerlMol

2003–Present

Perl Modules for Computational Chemistry and Chemoinformatics. Available in CPAN; with subscribers in over 20 pharmaceutical companies. Languages used: Perl. Lines of Code (LOC, not counting whitespace, comments, or documentation: ca. 6000).

AnnoCPAN

2005–Present

A web application that presents the documentation for every module on CPAN and allows users to add annotations on the margin. Sponsored by a Perl Foundation grant. Languages used: Perl, JavaScript, SQL. LOC: 2000.

dmoz.org

2002–2006

Developed search engines, anti-spam filters, and other tools for internal use. Languages used: Perl, C, JavaScript, SQL. LOC: 2000.

OSET

2000–2001

Organic Synthesis Exploration Tool. An educational program for retrosynthetic analysis. Languages used: C, Java, JavaScript. LOC: 10,000.

Affiliations**American Chemical Society**

2001–Present

Swiss Chemical Society

2007–Present

Yale Mexican Student Organization

Vice President

2004–2006

CPAN

User ID: ITUB

2003–Present

Languages

English (fluent), Spanish (native), French (basic), German (basic).

Last modified September 2007.