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# JORGE AGUILERA IPARRAGUIRRE

## EXPERIENCE

### **POST-DOCTORAL ASSOCIATE, MASSACHUSETTS INSTITUTE OF TECHNOLOGY**

CAMBRIDGE, MA SEPT 2010 - AUG 2013

DEPARTMENT OF CHEMICAL ENGINEERING, PROFESSOR W.H. GREEN GROUP

- Provide thermochemical data to assist in the creation of models to analyze the behavior of energy sources.
- Expert at determining the appropriate data sources for changing challenges, in particular, in the estimation of accuracy and errors from quantum calculations.
- Generate summary reports on the status of different projects and communicate with appropriate project partners and collaborators.
- Mentorship of graduate students including teaching the use of quantum chemistry tools to obtain data, permanent monitoring of students' progress, and ongoing assessment of students' understanding of computational tools.

### **POST-DOCTORAL ASSOCIATE, KARLSRUHE INSTITUTE OF TECHNOLOGY**

KARLSRUHE, GERMANY, APRIL 2009 - AUG 2010

DEPARTMENT OF PHYSICAL CHEMISTRY, PROFESSOR WIM KLOPPER, CHAIR OF THEORETICAL CHEMISTRY

## EDUCATION

### **DOCTORATE, MAGNA CUM LAUDE, KARLSRUHE INSTITUTE OF**

**TECHNOLOGY, KARLSRUHE, GERMANY FEB 2004 - MARCH 2009**

DEPARTMENT OF PHYSICAL CHEMISTRY, CHAIR OF THEORETICAL CHEMISTRY

- *Thesis*: "Ab initio calculations of hydrocarbon thermochemistry and reaction kinetics." First ever application of explicitly correlated methods (R12, F12) in the realm of kinetics.
- *Advisor*: Professor Wim Klopper, recipient of the Medal of the International Academy of Quantum Molecular Science and the Hans-G.A.-Hellmann Prize
- *Teaching Responsibilities*: Lecture laboratory on physical chemistry. Graded lab reports and provided laboratory exams. Assistant in programming course on Fortran 90.
- *Mentoring*: Introduced undergraduate students to quantum chemistry with 6-8 week-long projects that used different tools to obtain relevant data.
- *Academic stays abroad*:
  - University Paul Cezanne, Aix-Marseille III, France, in the Group of Theoretical Chemistry and modelization with Dr. Yannick Carissan September 2009.
  - University of Crete, Greece, in the Theoretical and Computational Chemistry group with Prof. George Frudakis April 2007.

- National University of Ireland, Galway, Ireland, in the Combustion Chemistry Centre with Prof. John Simmie and Henry Curran November 2006 and December 2007.
- *Other courses:* Fortran 90, Dynamical Electron Correlation, Numerical methods, and Relativistic effects

**M.S., MAGNA CUM LAUDE, UNIVERSIDAD DE ZARAGOZA, SARAGOSSA, SPAIN** SEPT 2001 - SEPT 2003  
DEPARTMENT OF PHYSICAL CHEMISTRY AND ORGANIC CHEMISTRY, GROUP OF HETEROGENEOUS CATALYSIS

- *Thesis:* “Applications of theoretical tools to the study of hetero-Diels-Alder reactions with dithioesters”
- *Advisor:* CSIC Prof. Jose Ignacio Garcia Laureiro

**B.S., UNIVERSIDAD DE ZARAGOZA, SARAGOSSA, SPAIN** SEPT 1996 - SEPT 2001

- *Major:* Chemistry; *Minor:* Organic Chemistry

## PUBLICATIONS

Quantum Chemical calculations focused on the study of novel fuel sources including bio-fuel and military applications

- A. Jalan, I. Alecu, R. Meana-Pañeda, J. Aguilera-Iparraguirre, K. Yang, S. Merchant, D. Truhlar and W. Green, New pathways for formation of acids and carbonyl products in low-temperature oxidation, the Korcek decomposition of ketohydroperoxides, *J. Am. Chem. Soc.*, 135(30), 11100-11114, **2013**
- V. V. Kislov, A. M. Mebel, J. Aguilera-Iparraguirre, W. H. Green, Reaction of Phenyl Radical with Propylene as a Possible Source of Indene and Other Polycyclic Aromatic Hydrocarbons: An Ab Initio/RRKM-ME Study, *J. Phys. Chem. A*, 116, 4176-4191 **2012**
- G. Magoon, J. Aguilera-Iparraguirre, W. Green, J. Lutz, P. Piecuch, O. Oluwole and H-W. Wong, Detailed chemical kinetic modeling of JP-10 (exo-tetrahydrodicyclopentadiene) high temperature oxidation: Exploring the role of biradical species in initial decomposition steps, *Int. J. Chem. Kin.*, 44, 179-193, **2012**
- R. I. Kaiser, D. S. N. Parker, M. Goswami, F. Zhang, V. V. Kislov, A. M. Mebel, J. Aguilera-Iparraguirre, W. H. Green, Crossed beam reaction of phenyl and D5-phenyl radicals with propene and deuterated counterparts-competing atomic hydrogen and methyl loss pathways, *Phys. Chem. Chem. Phys.*, 14, 720-729 **2012**
- S. H. Dürrstein, M. Olzmann, J. Aguilera-Iparraguirre, R. Barthel and W. Klopper, The phenyl + phenyl reaction as pathway to benzynes: An experimental and theoretical study, *Chem. Phys. Lett.*, Accepted **2011**
- W. Klopper, R. A. Bachorz, D. P. Tew, J. Aguilera-Iparraguirre, Y. Carissan and C. Hattig, Accurate coupled-cluster calculations of the reaction barrier heights of two CH<sub>3</sub>+CH<sub>4</sub> reactions, *J. Phys. Chem. A*, 113, 11679-11684 **2009**
- J. Aguilera-Iparraguirre, H.J. Curran, W. Klopper and J.M. Simmie, Accurate benchmark calculation of the reaction eight for hydrogen abstraction by the

hydroperoxyl radical from methane; Implications for  $C_nH_{2n+2}$  where  $n=2-4$ , *J. Phys. Chem. A*, 112, 7047-7054 **2008**

- J. Aguilera-Iparraguirre, A. D. Boese, W. Klopper and B. Ruscic, Accurate ab-initio computation of thermochemical data for  $C_3H_x$  ( $x=0, \dots, 4$ ) species, *Chem. Phys.*, 346, 56-58 **2008**
- J. Aguilera-Iparraguirre, H. J. Curran, W. Klopper and J. M. Simmie, Calculation of reaction rates for hydrogen abstraction by the hydroperoxyl radical from C1 through C4 hydrocarbons, *Proceedings of the European Combustion Meeting* **2007**
- J. Aguilera-Iparraguirre and W. Klopper, Density functional theory study of the formation of naphthalene and phenanthrene from reactions of phenyl with vinyl- and phenylacetylene, *J. Chem. Theor. Comp.*, 3, 139-145 **2007**
- +4 in preparation

#### MEETINGS AND CONFERENCES

- The 7<sup>th</sup> International Conference in Chemical kinetics, Cambridge, MA (USA) 1-14 July, 2011.
- European Combustion Meeting 2007, Chania (Greece), 11-13 April, 2007. With the poster contribution: Calculation of Reaction Rates for Hydrogen Abstraction by the Hydroperoxyl Radical from C1 through C4 Hydrocarbons.
- Workshop of the SPP 1145 "Highly Accurate Molecular Electronic-Structure Theory", Bad Herrenalb (Germany), 22-24 March 2007. With the poster contribution: Calculation of Reaction Rates for Hydrogen Abstraction by the Hydroperoxyl Radical from C1 through C4 Hydrocarbons
- 42nd Symposium on Theoretical Chemistry STC 2006, Erkner (Germany), 3-6 September 2006. With the poster contribution: Accurate Coupled-Cluster energies of  $C_xH_y$  ( $x=1, \dots, 3; y=0, \dots, 4$ )
- Seminar on Theoretical Chemistry of Karlsruhe, Mainz and Stuttgart Research Groups, Hirschegg (Austria), January 2006.
- Seminar on Theoretical Chemistry of Karlsruhe, Mainz and Stuttgart Research Groups, Hirschegg (Austria), February 2005.
- International Conference in Honor of Reinhardt Ahlrichs Computational Tools for Molecules, Clusters, and Nanostructures Karlsruhe (Germany), 23-26 January 2005
- Research Groups Meeting from Karlsruhe and Mainz, Mainz (Germany), 11 December 2004. With the oral presentation contribution: Accurate thermochemistry of the dissociation of Propyne.

#### COURSES

- Winter-Semester Seminar on quantum chemistry. Numerical methods, with the oral presentation contribution: Diagonalising big matrices, 9 December 2009.
- Winter-Semester Seminar on quantum chemistry. Relativistic effects, with the oral presentation contribution: Breit Interaction, 5 February 2007.
- A Tutorial on Dynamical Electron Correlation, Zurich (Switzerland), 2-4 October 2006
- Modulares Programmieren in FORTRAN 90, 31 July-4 August 2006
- Winter-Semester Seminar on quantum chemistry. Density Functional Theory, with the oral presentation contribution: Density Matrices, 14 November 2005.
- Numerische Methoden in der Chemie in FORTRAN, 10-21 October 2005

- European Summerschool in Quantum Chemistry, Torre Normanna (Italy), 4-17 September 2005. With the poster contribution: Reaction mechanisms and rates for aromatic hydrocarbon radicals from DFT calculations

#### **OTHER INTERESTS**

Always interested in sports, I have, since coming to the United States learned to ice-skate and attempted to play ice-hockey (the puck of my first goal is one of my most beloved possessions). Also started a love-hate relationship with golf. At MIT I discovered the field of Sport Analytics and I'm doing my best to get up to speed. Assisting the recently founded Spain@MIT association in exposing Spanish culture to the Boston community.