



Dr. Carlos Gonzalez's Bio

Dr. Gonzalez received his Ph.D in Theoretical Chemistry at Wayne State University, in 1990. He then moved in 1991 to Pittsburgh where he worked as a postdoctoral associate in Carnegie Mellon University under the supervision of Prof. John A. Pople, Nobel Laureate in Chemistry 1998. He joined the Chemical Sciences and Technology Laboratory at the National Institute of Standards and Technology (NIST) in 1997 as a Research Chemist, after spending 5 years as a Research Specialist at the Pittsburgh Supercomputing Center, Carnegie Mellon University. Dr. Gonzalez has extensive experience in the development and implementation of modern ab initio quantum chemical methodologies and their application to a wide variety of chemical problems. His work leading to the development of an efficient methodology to compute minimum energy reaction paths within the Intrinsic Reaction Coordinate formalism has been widely cited in the open literature (over 5,000 citations, according to the Citation Index). Dr. Gonzalez was the founder of the NIST's Center for Theoretical and Computational Nanosciences, which he directed for 3 years. The Center's mission was essentially: (1) To develop, implement and validate efficient and reliable theoretical methodologies and computational infrastructure required for understanding chemistry, physics, and biology at the nano-scale, (2) Serve as a center for collaboration with scientists in industry, academia and national labs to efficiently apply theory and simulation in the field of nanotechnology and (3) Help industry identify and utilize effective computational solutions to problems limiting realization of the promise of nanotechnology. Dr Gonzalez has published over 100 papers in the area of quantum chemistry, and is one of the co-authors of the Gaussian suite of programs, the most popular ab initio electronic structure package currently available. Dr. Gonzalez's research interests focus in the development and implementation of reliable and efficient quantum chemistry methodologies in the study of physical and chemical properties of a wide variety of chemical systems, chemical reactivity, long-range interactions in molecules and solids, and nanotechnology. For the past eight years, he has also been involved in the development of efficient computational tools for data analysis and chemical informatics as applied to areas such as materials by design, climate science and chemical reactivity. Dr. Gonzalez is the recipient of the 2005 Department of Commerce Brown Medal and more recently, the 2007 Science Spectrum Magazine's Minorities in Research Science Emerald Honor "for his exemplary performance in the area of research leadership". Dr. Gonzalez is currently the Chief of the Chemical Sciences Division at NIST.