Co-hosted by Purdue Quantum Science and Engineering Institute and Discovery Park

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Effective Integration of NIST Reference Data, Reference Materials, and Informatics in Support of Science and Technology

The mission at the National Institute of Standards and Technology (NIST) is "To promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve our quality of life." Being the National Metrology Laboratory of the United States, NIST scientists are responsible for providing critical advancements in measurement science to address the nation's needs for reliable and accurate metrology and traceability, transferring new measurement technology to the U.S. and international customers and users.

In support of this mission, NIST provides a wide variety of measurement services encompassing four important programs: Calibrations, Standard Reference Materials® (SRMs), Standard Reference Data (SRD), and Laboratory Accreditation. In particular, the SRMs program at NIST includes over 1,300 artifacts traceable to national standards suitable for in situ self-calibration and methods validation, while the SRD program includes a large and diverse amount of data archived and critically evaluated that is widely disseminated in printed and/or electronic media.

Impressive scientific advances during the past two decades, specially in the areas of the physical/materials sciences, nanotechnology, biomedicine, and informatics (machine learning and artificial intelligence), have made it clear that most of the current scientific and technological activities have become information-driven and data-centric endeavours that will pose significant demands for more accurate and reliable data as well as critical challenges related to the management of massive amounts of data produced by measurements and simulations, the so-called "data deluge" or "data singularity." This is particularly true in the areas of clinical diagnoses, food quality and safety, environmental sciences, and petroleum chemistry, where a new paradigm-shift involving the seamless integration of reference materials and reference data seems to be the logical way forward for information providers and metrology laboratories given the ever-increasing demand for large and complex data sets. To achieve this goal, novel dissemination models (such as modern interactive databases and scientific workflows), as well as data information tools must be implemented, where databases and data analysis tools covering a wide variety of physical and chemical properties of particular reference materials could be made available to scientists and engineers. In addition, these tools should be interactive so that scientists could submit data related to new properties not originally contained in the databases or in the Certificate of Analysis for the reference materials. At the end, entire scientific communities supporting particular reference materials will be created making the metrology laboratories supporting these activities *scientific information brokers* rather than just *data providers*.

In this talk, a general description of NIST's SRM program will be provided, highlighting some examples related to environmental science, clinical diagnoses and petroleum chemistry. In addition, issues related to the effective integration of reference data with reference materials and modern informatics tools will be discussed, as well as ideas leading to the development of novel NIST measurement services in chemistry.

Dr. Carlos Gonzalez

Dr. Gonzalez received his Ph.D in Theoretical Chemistry from Wayne State University in 1990. In 1991 he moved to Pittsburgh where he worked as a postdoctoral associate at Carnegie Mellon University under the supervision of Prof. John A. Pople, 1998 Nobel Laureate in Chemistry. 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 five 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 (more than 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 three 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 more than 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 on 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.

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