

NWChem Delegation Members of EMSL PNNL

Coordinators [Dr. Zhong Jin \(CNIC, CAS\)](#) & [Prof. Jun Li \(Tsinghua Chemistry\)](#)



Name: **Dr. William A. Shelton**

Title: Associate Director, Molecular Sciences Computing

Presentation Title: [EMSL Current and New directions: Scientific Innovation through Integration](#)

Brief Resume:

Bill Shelton is currently the Associate Director for Computing in the Environmental Molecular Sciences Laboratory (ESML) at the Pacific Northwest National Laboratory (PNNL). Prior to joining ESML in September 2010, Bill was in the Computing and Computational Sciences Directorate at Oak Ridge National Laboratory for the past 18 years. Bill received his Ph.D in Theoretical Condensed Matter Physics from the University of Cincinnati in 1989. He then received a National Academy of Sciences National Research Council Post doctoral fellowship. After his NRC post doctoral fellowship, Bill joined the Computing and Computational Sciences Directorate at Oak Ridge National Laboratory (ORNL) where he continued to work on superconductivity, disordered magnetic alloys, surfaces and interfaces in several DOE Grand Challenge and Scientific Discovery through Advanced Computing projects for the past 18 years. Bill has won several high performance computing awards including 3 Gordon Bell Awards (2001 Special Honorable Mention, 1998, 1990), a Computerworld Smithsonian Laureate Award (2000), a Cray Gigaflop Award (1990) and 3 Gold Medal High Performance Computing Challenge Awards (1995,1996), and in addition he has won 2 ORNL Scientific Achievement Awards (1991,1994) and a ORNL Division Director's Award (1990,1993).



Name: **Dr. Wibe Albert de Jong**

Title: Capability Steward High Performance Software Development, EMSL, Pacific Northwest National Laboratory

Presentation Title: [Modeling the Chemistry of Actinide Species in the Environment](#)

Brief Resume:

Dr. de Jong is a scientist at the EMSL for 10 years. EMSL is a national user facility located at Pacific Northwest National Laboratory (PNNL). At EMSL he is the Capability Steward leading the development of the NWChem computational chemistry software. In addition, Dr. de Jong leads an computational actinide chemistry research program funded by the US Department of Energy and various funded projects in the development of high performance computational chemistry software. Before becoming a staff member at PNNL, de Jong was a Postdoctoral Researcher at PNNL. He received his education in the Netherlands where he earned a PhD in Theoretical Chemistry and a MS in Physical Chemistry from the University of Groningen and a BS in Chemical Engineering from the Technical College of Leeuwarden. He has published 56 peer reviewed journal articles plus 3 book chapters, and has presented 20 invited lectures. He has mentored 3 postdoctoral fellows. Dr. de

Jong's research interests are actinide chemistry, the development of highly scalable parallel computational chemistry algorithms, and the integration of modeling and experiment.



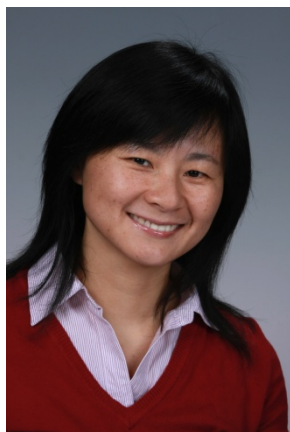
Name: **Dr. Niranjan (Niri) Govind**

Title: Senior Scientist

Presentation Title: [Excited-State Studies in Molecules and Materials](#)

Brief Resume:

Dr. Govind did his graduate work with Prof Hong Guo at McGill University in Montreal, Canada and post-doctoral work with Prof. Emily Carter at UCLA, Los Angeles. He has 15 years experience working on the development and application of electronic structure methods. Dr. Govind is presently a Senior Scientist in the High Performance Software Development Group at the Environmental Molecular Sciences Laboratory (EMSL) at the Pacific Northwest National Laboratory (PNNL). He is a member of the NWChem software development team and is responsible for the development of the DFT and TDDFT modules in the NWChem quantum chemistry package. His research interests include: development of methods and algorithms in electronic structure theory focusing on DFT and TDDFT, ground and excited-state properties of molecules and materials, orbital-free DFT, embedding methodologies and optimization algorithms. Prior to joining EMSL 3 years ago, Dr. Govind spent 7 years in industry working for Accelrys, Inc in San Diego, CA where he worked on various electronic structure packages (CASTEP, DMol³, VAMP) and has made significant contributions to them.



Name: **Dr. Ping Yang**

Title: Senior Research Scientist at Molecular Science Computing of EMSL

Presentation Title: [Convergence of Theory and Experiment through Electronic Structure Calculations](#)

Brief Resume:

Ping Yang received her master degree in computer science in 2004 and doctorate in computational chemistry in 2005 from Michigan Technological University. From 2006 to 2008, she was Seaborg Postdoctoral Fellow working with Richard Martin and P. Jeffrey Hay at Los Alamos National Laboratory (LANL). Since 2008, she joined the Environmental Molecular Sciences Laboratory at Pacific Northwest National Laboratory (PNNL) as a senior research scientist. Her experience includes fundamental structural properties, bonding interactions, and reaction mechanisms in organoactinide molecules, hydrogen bonding networks in biological complexes, and studies of the electronic structure of disordered organic electronic materials. Dr. Yang's current research interests focus on theoretical and computational studies of actinide chemistry, catalysis chemistry, biological complexes, and nanomaterials.