NWChem Delegation Members of EMSL PNNL

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

Name: **Allison Campbell**
Title: Director of EMSL, Pacific Northwest National Laboratory
Brief Resume:
Dr. Allison A. Campbell is the Director of EMSLð the Environmental Molecular Sciences Laboratory. Her primary responsibility is to lead EMSL in maintaining and growing its reputation as a premier scientific user facility. EMSL provides integrated experimental and computational resources for discovery and technological innovation in the environmental molecular sciences to support the needs of DOE and the nation. More than 700 scientists from around the world access EMSLôs capabilities each year. Campbell led the investment of more than $100 million in new capabilities that are coming online and will be available to the global scientific community.
Dr. Campbell is nationally recognized for her contributions towards materials development through her research in the field of biomaterials. Dr. Campbell is credited with co-inventing a bio-inspired process to "grow" a bioactive calcium phosphate layer, from the molecular level, onto the surfaces of artificial joint implants (total hip and knee) to extend implant life and reduce rejection. She is also recognized for her work in understanding the role of proteins in biomineralization process such as tooth formation and decay. She has authored numerous peer reviewed technical papers, been an invited speaker at national and international meetings, and has several patents based upon her research. Additionally, Dr. Campbell is an avid promoter of science education, sharing her enthusiasm for science with young students through a number of hands-on education programs.

Name: **Dr. Wibe Albert de Jong**
Title: Capability Steward High Performance Software Development, EMSL, Pacific Northwest National Laboratory
Brief Resume:
Dr. de Jong is a scientist at the EMSL for 12 years. EMSL is a national user facility located at Pacific Northwest National Laboratory (PNNL). At EMSL he is the Capability Stewards 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 Jongôs 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
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 17 yearsô 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 5 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, $DMol_3$, VAMP) and has made significant contributions to them.

Name: **Dr. Ping Yang**
Title: Senior Research Scientist at Molecular Science Computing of EMSL
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.

The invited speakers will provide pedagogical and expository lectures on the methods that they use, complemented by hands-on sessions*. The format allows plenty of time for discussions.

(*Participants need to bring their own laptop for the hands-on sessions.)