

Accolades

Three EMSL Users Selected as Inaugural Visiting Scientists

Three longtime users of the Department of Energy's EMSL have been appointed as participants of EMSL's Wiley Visiting Scientist Program, which is designed to recognize, reward, and encourage distinguished scientists to come to EMSL for extended periods of time and make significant contributions to the EMSL user program by providing input to and recommendations on the path forward for EMSL.

- Walter Ermler is professor of chemistry at the University of Texas at San Antonio. At EMSL, he will work to integrate his CRENB spin-orbit operators with EMSL's NWChem software suite basis set and the EMSL Basis Set Exchange Library for the entire periodic system. The availability of these spin-orbit potentials in NWChem will directly support geochemistry and subsurface science research by enabling calculations that can provide more accurate results for those studying the structures and reaction mechanisms of heavy-element contaminants at various interfaces at the molecular scale. He will also develop collaborations in the area of modeling the electronic structure and spectroscopic properties of trans-uranium molecules and clusters using highly accurate relativistic methodologies.
- Ian Farnan is on the faculty of the Department of Earth Sciences at University of Cambridge. During his fellowship, Farnan will work to develop the next stage of radiological magic-angle spinning nuclear magnetic resonance capability at EMSL, encompassing higher sample rotation speeds and variable temperature operation. He has been instrumental in past collaborations with EMSL to develop the technology and sample handling protocol for high-resolution, solid-state NMR experiments on plutonium, and his work has led to notable findings in the area of radiation damage produced in zircon ceramics.
- Alex Shluger is on the Department of Physics and Astronomy faculty at University College London. At EMSL, he will expand on his work in laser desorption from metal oxides to include new opportunities for connecting topographic surface features on oxides to their spectroscopic and chemical properties and, therefore, develop an understanding of photo-induced and chemical processes for sculpting nanoscale metal oxide surfaces. Such surfaces could be beneficial for catalytic and energy applications. Part of this research will involve exchange and implementation of *ab initio* codes developed by Shluger's research team and EMSL's NWChem code.



Walter Ermler



Ian Farnan



Alex Shluger

Applications for the Wiley Visiting Scientist Program are accepted quarterly, and appointments include a stipend for travel and per diem. For more information, see http://www.emsl.pnl.gov/news/awards/visiting_scientist.jsp.